



Radioactive Waste Isolation in Salt: Special Advisory Report on the Status of the Office of Nuclear Waste Isolation's Plans for Repository Performance Assessment

J. D. Ditmars, E. W. Walbridge, D. M. Rote,
W. Harrison, and C. L. Herzenberg

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**RADIOACTIVE WASTE ISOLATION IN SALT:
SPECIAL ADVISORY REPORT ON THE STATUS OF THE
OFFICE OF NUCLEAR WASTE ISOLATION'S PLANS
FOR REPOSITORY PERFORMANCE ASSESSMENT**

by

**J.D. Ditmars, E.W. Walbridge, D.M. Rote,
W. Harrison, and C.L. Herzenberg**

**Energy and Environmental Systems Division
Geoscience and Engineering Group**

October 1983

work sponsored by

**U.S. DEPARTMENT OF ENERGY
Salt Repository Project Office
Office of Civilian Radioactive Waste Management**

FOREWORD

Documents are being submitted to the Salt Repository Project Office (SRPO) of the U.S. Department of Energy (DOE) by Battelle Memorial Institute's Office of Nuclear Waste Isolation (ONWI) to satisfy milestones of the Salt Repository Project of the Civilian Radioactive Waste Management Program. Some of these documents are being reviewed by multidisciplinary groups of peers to ensure DOE of their adequacy and credibility. Adequacy of documents refers to their ability to meet the standards of the U.S. Nuclear Regulatory Commission, as enunciated in 10 CFR 60, and the requirements of the National Environmental Policy Act and the Nuclear Waste Policy Act of 1982. Credibility of documents refers to the validity of the assumptions, methods, and conclusions, as well as to the completeness of coverage.

Since late 1982, Argonne National Laboratory has been under contract to DOE to conduct multidisciplinary peer reviews of program plans and reports covering research and development activities related to siting and constructing a high-level nuclear waste repository in salt.

In response to an earlier Argonne peer review report* critiquing ONWI's *Preliminary Performance Assessment Plan for a Nuclear Waste Repository* and *Verification and Validation Plan for Performance Assessment Technology for a Nuclear Waste Repository in Salt*, DOE requested that Argonne provide guidance on combining these two documents and on improving their quality. Particular attention was to be paid to upgrading the status reports on the various computer codes selected by ONWI for use in repository performance assessment.

A draft of this special advisory report was sent to SRPO on October 10, 1983.

*W. Harrison et al., *Radioactive Waste Isolation in Salt: Peer Review of the Office of Nuclear Waste Isolation's Plans for Repository Performance Assessment*, Argonne National Laboratory Report ANL/EES-TM-246 (May 1984).

PREVIOUSLY PUBLISHED REPORTS IN THE SERIES

"RADIOACTIVE WASTE ISOLATION IN SALT"

- ANL/EES-TM-242 Peer Review of the Office of Nuclear Waste Isolation's
Geochemical Program Plan (Feb. 1984)
- ANL/EES-TM-243 Peer Review of the Office of Nuclear Waste Isolation's
Socioeconomic Program Plan (Feb. 1984)
- ANL/EES-TM-246 Peer Review of the Office of Nuclear Waste Isolation's
Plans for Repository Performance Assessment (March 1984)
- ANL/EES-TM-254 Peer Review of the Office of Nuclear Waste Isolation's
Reports on Preferred Repository Sites within the Palo Duro
Basin, Texas (June 1984)

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Microfiche copies of the following unpublished reports are attached to the inside back cover of this report:

1. Office of Nuclear Waste Isolation, *Preliminary Performance Assessment Plan for a Nuclear Waste Repository in Salt*, Battelle Memorial Institute, Columbus, Ohio (April 1983).
2. Office of Nuclear Waste Isolation, *Verification and Validation Plan for Performance Assessment Technology for a Nuclear Waste Repository in Salt*, Battelle Memorial Institute, Columbus, Ohio (June 24, 1983).

AUTHORS OF CODE STATUS SUMMARIES

<u>Name</u>	<u>Computer Code(s)</u>
J.D. Ditmars	GRESS LAYFLO MMT
E.W. Walbridge	DOT FE3DGW HEATING6 NETFLO SALT4 SPECTROM-58 STAFAN STEALTH TEMP VISCOT
D.M. Rote	CFEST EQ3/EQ6 FTRANS GEOTHER ORIGEN2 PHREEQE SWENT THAC-SIP-3D TRIPM WAPPA
W. Harrison	FFSM
C.L. Herzenberg	DACRIN PABLM UCB-NE-n

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ABSTRACT

Repository performance assessment is analysis that identifies events and processes that might affect a repository system for isolation of radioactive waste, examines their effects on barriers to waste migration, and estimates the probabilities of their occurrence and their consequences. In 1983 Battelle Memorial Institute's Office of Nuclear Waste Isolation (ONWI) prepared two plans -- one for performance assessment for a waste repository in salt and one for verification and validation of performance assessment technology. At the request of the U.S. Department of Energy's Salt Repository Project Office (SRPO), Argonne National Laboratory reviewed those plans and prepared this report to advise SRPO of specific areas where ONWI's plans for performance assessment might be improved.

This report presents a framework for repository performance assessment that clearly identifies the relationships among the disposal problems, the processes underlying the problems, the tools for assessment (computer codes), and the data. In particular, the relationships among important processes and 26 model codes available to ONWI are indicated. A common suggestion for computer code verification and validation is the need for specific and unambiguous documentation of the results of performance assessment activities.

A major portion of this report consists of status summaries of 27 model codes indicated as potentially useful by ONWI. The code summaries focus on three main areas: (1) the code's purpose, capabilities, and limitations; (2) status of the elements of documentation and review essential for code verification and validation; and (3) proposed application of the code for performance assessment of salt repository systems.

1 INTRODUCTION

1.1 BACKGROUND

In an earlier report critiquing the Office of Nuclear Waste Isolation's (ONWI's) program plans for salt repository performance assessment (Harrison et al., 1984), Argonne peer review panels recommended that the two relevant ONWI plans (Office of Nuclear Waste Isolation, 1983a, 1983b)* be combined into a single document. The U.S. Department of Energy's (DOE's) Salt Repository Project Office accepted this recommendation and directed Argonne to provide a framework within which such a combination could be carried out. The office also requested that Argonne suggest how the various parts of the ONWI plans could be improved, with emphasis on the status reports on the various codes being developed for repository performance assessment.

The authors of the present report were members of peer review panels for either one or both of the two ONWI plans, with the exception of C.L. Herzenberg. Authors did not contact ONWI personnel nor have they been involved in any programs sponsored by DOE or directed by ONWI such that their participation in the preparation of this report could be construed as a conflict of interest.

1.2 PURPOSE AND SCOPE

The first objective of this report is to justify the need for additional overview information in a combined report. In particular, clarification is needed on (1) the relationships between the behavior of the repository system and the processes being modeled, (2) the nature of the links between codes, and (3) the verification and validation aspects of repository performance assessment. The second objective is to provide realistic and informative summaries of the status of computer codes selected by ONWI for performance assessment.

Repository performance assessment requires more than assembling relevant computer codes. The technical community must be informed of the framework for performance assessment, including the nature of the scientific and engineering problems to be treated, the specific processes underlying the problems, how the processes will be modeled, and the degree to which a series of linked models will represent the overall system under consideration. The discussion of overview material in this report is restricted to postclosure performance assessment, with all of the processes important for the waste package, repository, and far-field environments being covered. The summaries of the status of the model codes selected by ONWI (Office of Nuclear Waste Isolation, 1983b) for postclosure assessment are not meant to be the final word on the subject but are sufficiently complete for easy incorporation into a combined document. They follow an Argonne format that covers more subjects and treats them in greater detail than the status reports in the ONWI Verification and Validation Plan (VVP). In particular, they

*Microfiche copies of the unpublished referenced reports are attached to the inside back cover of this report.

cover in more detail the degree of code verification and the quality and appropriateness of the documentation with respect to NUREG-0856 (Silling, 1983) requirements. Also discussed more realistically is the suitability of the codes for application to salt repository performance assessment.

1.3 DEFINITIONS

The following terms are used in this report as defined below.

1. Performance assessment. Analysis to identify events and processes that might affect a repository system for isolation of radioactive waste, to examine their effects on barriers to waste migration, and to estimate the probabilities of their occurrence and their consequences. The analysis need not evaluate risks from all identified events and processes. However, it should provide reasonable assurance that the risks from those that are not evaluated are small in comparison with the risks from those that are.
2. Verification. Testing and evaluation to assure that a computer code correctly performs the operations specified in a mathematical model.
3. Validation. Testing and evaluation to assure that a model as embodied in a computer code is a correct representation of the process or system being modeled.

1.4 REFERENCES FOR SECTION 1

Harrison, W., et al., *Radioactive Waste Isolation in Salt: Peer Review of the Office of Nuclear Waste Isolation's Plans for Repository Performance Assessment*, Argonne National Laboratory Report ANL/EES-TM-246 (May 1984).

Office of Nuclear Waste Isolation, *Preliminary Performance Assessment Plan for a Nuclear Waste Repository in Salt*, Battelle Memorial Institute, Columbus, Ohio, unpublished manuscript (1983a).

Office of Nuclear Waste Isolation, *Verification and Validation Plan for Performance Assessment Technology for a Nuclear Waste Repository in Salt*, Battelle Memorial Institute, Columbus, Ohio, unpublished manuscript (1983b).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (1983).

2 FRAMEWORK FOR PERFORMANCE ASSESSMENT

Repository performance assessment has a framework within which items like computer codes and verification and validation exercises are supporting members. Reviewers of ONWI's Performance Assessment Plan (PAP) and VVP concluded, in part, that the plans are not likely to be fully understood or appreciated because the performance assessment framework is not clearly presented (Harrison et al., 1984). This report provides a perspective on the framework for performance assessment and a few of its essential features so that revisions of the PAP and VVP documents and related future documents will meet DOE program objectives.

The performance assessment framework is shown schematically in Fig. 1. Arrows indicate the general direction of decision making and information flow during the assessment process. The first step is identification of the problems, both engineering and scientific, that require assessment for the postclosure period. Many of these problems have already been identified in the PAP document. Once the problems have been identified, the fundamental processes (physical, chemical, and biological) governing the problems must be identified, and most importantly, the relationships among these processes and problems must be clearly established. This second critical step appears to be either absent or not easily recognized in the PAP and VVP documents.

Given the relationships among the technical problems and the governing processes, certain tools are necessary for using information on the processes to analyze the problems. These tools are the mathematical models and related computer codes. Many of these tools are identified in PAP and VVP and are described in individual code documents. Their relationships to each other must be understood before they can be used effectively as a set of tools. The relationships among the codes have not been well documented in either PAP or VVP.

The quality of the codes and their suitability for performance assessment are determined through verification and validation, which were addressed, although inadequately, in VVP. An element essential to the performance assessment framework is accurate reporting of the status of

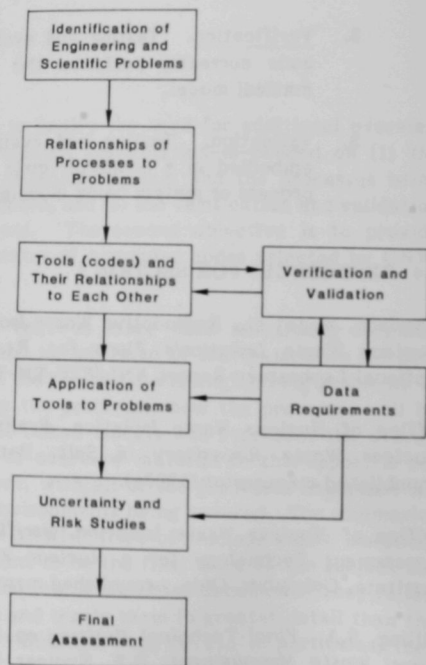


FIGURE 1 Framework for Performance Assessment

verification and validation activities for each code. The initial attempt at status reporting in VVP was judged by the peer review panel to be inadequate.

Once codes have been found adequate for specific situations, they can be applied to the problems initially identified. However, application procedures are not yet documented. Such application requires not only code validation within the range of parameters appropriate to the specific problem but also design- and site-specific data for the application. Thus, the performance assessment framework must include consideration of the data requirements in the context of the codes and anticipated applications. The links among individual models, their input data, and possible applications have not been addressed. Before assessments are completed, uncertainty and risk should be evaluated through sensitivity studies. The scope and procedures for such studies have not yet been documented, but they must be related to data requirements and model capabilities.

In Sec. 2, we address those aspects of the framework for performance assessment that lie between problem identification and verification and validation that have not been adequately addressed in the PAP and VVP documents. The general problems and processes are discussed in Sec. 2.1, and the relationships among the problems, processes, and codes are outlined in Sec. 2.2. Examples of relationships of codes to each other are provided in Sec. 2.3. (Summaries of individual codes and their status are given in Sec. 3.) Essential issues of verification and validation not specifically addressed in the VVP document are highlighted in Sec. 2.4.

2.1 DESCRIPTION OF GENERAL PROCESSES

Our studies of the PAP, VVP, and individual code documents indicate that there is insufficient description and discussion of the processes that might affect the release of radionuclides to the biosphere. Only from such descriptions and discussions of relevant processes (physical, chemical, and biological) will it become apparent what codes will be required and what questions they should address. In other words, an understanding of the processes is essential to an understanding of performance assessment. In the PAP, VVP, and code documents, the codes are emphasized, often without relating them to the processes. The process framework is what holds the collection of codes together; without it, the codes are just a vaguely related collection. In addition, development of an overall process framework is the best way to identify processes that have been overlooked, processes that have been inadequately modeled, and processes that have negligible consequences.

We urge ONWI to develop simple physical and chemical descriptions of each of the processes related to the escape of radionuclides from the waste form, their transport by groundwater, and their entry into the biosphere. The time sequencing of the processes should also be described. Each process description should be accompanied by a discussion employing simple analytic solutions and "back-of-the-envelope" calculations to generate a good heuristic understanding of the process.

2.2 RELATIONSHIPS AMONG PROBLEMS, PROCESSES, AND CODES

To facilitate postclosure assessment of repository performance, the waste isolation system is divided into waste package, repository, and site subsystems. As decided by the U.S. Nuclear Regulatory Commission (NRC), the problems associated with performance of barriers to radioactive waste migration in each subsystem should be simulated by numerical modeling. Analysis of the results of simulations accomplished by state-of-the-art numerical models is a crucial step in providing NRC with the "reasonable assurance" of system safety required for repository licensing. Another crucial step is development of an overall physical picture, which provides a context for the individual processes and codes (see Sec. 2.1).

It is DOE's responsibility to simulate by numerical modeling the various processes that can affect the performance of a waste isolation system. These processes are displayed horizontally at the top of Table 1. Codes are listed vertically on the left. The processes are grouped from left to right in a roughly chronological sequence. The leftmost processes are those that relate to the waste package only, except for waste package corrosion, which is closely linked to radionuclide transport processes and is therefore grouped with those later processes. The first impacts of the stored waste are that each waste package generates heat and radioactivity, that heat flows within the waste package, and that the package is affected by the radiation and responds thermomechanically to the heat. These first processes are grouped under "Waste Package Processes." The code or codes that simulate these processes are indicated by x's in the columns beneath each process.

Heat generated in and around the waste package is conducted into the repository. The second group of processes has to do with the response of the dry repository to the heat from the waste packages. If there is no flow of groundwater to the repository, the first and second groups of processes cover the spectrum of what can happen.

If groundwater can flow to, or to and from, the repository, several additional processes need to be included. These processes are divided into three groups: (1) flow of water (not necessarily in salt) to or from the repository area, (2) flow of water through the salt repository, and (3) transport of radionuclides from the repository through the site, or far field. Within each of the five groups, the individual processes are displayed, as much as possible, in chronological sequence, with the earliest occurring process being the leftmost in each group.

2.3 EXAMPLES OF LINKAGE AMONG CODES

Panelists reviewing both the PAP and VVP documents recommended that details be provided on the sequential execution of individual process models, that is, on how the output of one model is input to the next. To demonstrate what the peer review panelists meant by providing examples of the linkages between codes, we decided to describe the DOT-VISCOT and SWENT-PABLM code links.*

TABLE 1. Processes that May Occur when Radioactive Waste is Stored in a Mined Underground Repository in Salt and the Codes that Model Those Processes

[illegible]

2.3.1 DOT to VISCOT Link

DOT (INTERA, 1983a, ONWI-420) is a two-dimensional, finite-element heat transfer code that uses linear and nonlinear thermal properties and time-dependent heat generation to predict temperatures as a function of time and position. VISCOT (INTERA, 1983b, ONWI-437) is a two-dimensional, finite-element code for calculating time-dependent, nonlinear deformations of a rock mass in response to geostatic and thermal stresses. The DOT to VISCOT link is shown in Fig. 2.

Certain of the inputs to VISCOT, namely, a description of system geometry and the mass density, are also inputs to DOT. The two-dimensional (planar or axisymmetric) temperature field constitutes the primary output from DOT and is one of the inputs into VISCOT. For the temperature field generated by DOT to be accepted as input by VISCOT, the DOT and VISCOT mesh geometries must be identical.

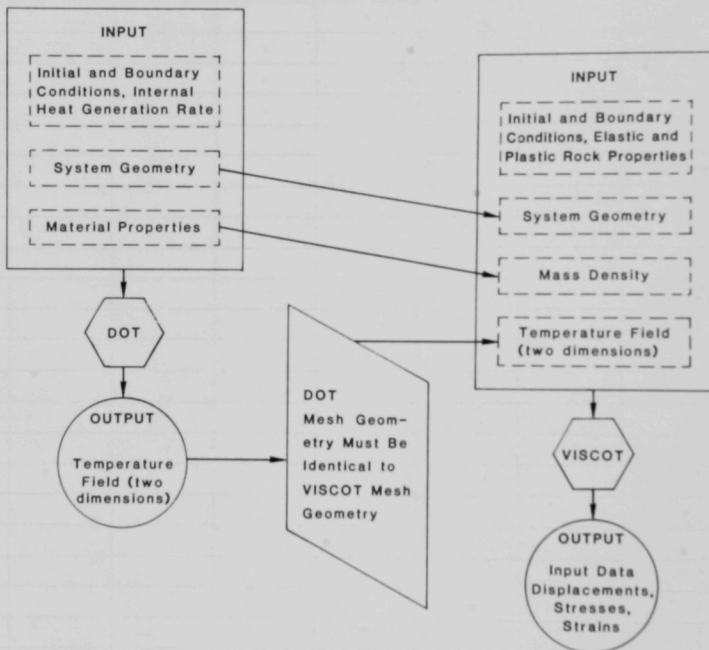


FIGURE 2 Information Flows from DOT to VISCOT

2.3.2 SWENT to PABLM Link

SWENT (INTERA, 1983c, ONWI-457) simulates the transient, three-dimensional transport through a heterogeneous geologic medium of fluid, energy, an inert component, and any number of radionuclides. The PABLM code (INTERA, 1983d, ONWI-446) estimates dose-to-man from radiation exposure and ingestion of radionuclides transported through aquatic and terrestrial pathways in the biosphere. As shown schematically in Fig. 3, the link between the pertinent processes of the two models is the flux of radionuclides (or radionuclide discharge rates) from the groundwater system to waters considered in PABLM.

Input to the aquatic pathway portion of PABLM requires information on release rates of radionuclides from groundwaters to rivers or other surface waters. Given the release rate from groundwater, the river flow rate, and the expected degree of mixing of the groundwater with the river, PABLM determines internal exposure to humans through consumption of fish, crustaceans, mollusks, water plants, and water; and external exposure to surface waters through boating and swimming and to shoreline sediments. SWENT can provide radionuclide release rates as output at each

computational block face, and if specified as input, release rates over large computational boundaries called biosphere discharge regions. As many as four such biosphere discharge regions can be designated for each SWENT computation, and release rates are provided at those boundaries in a form immediately compatible with the PABLM input requirement. Essential for the proper linkage between SWENT and PABLM is the careful structuring of SWENT geometry and the designation of biosphere discharge regions in SWENT such that the regions represent the intersections of the groundwater system with rivers, lakes, reservoirs, and wells, where input is required for PABLM.

Radionuclide transport information determined by SWENT can be channeled to PABLM via intermediate tape files. Data for four possible radionuclide discharge regions, such as a lake, stream, or groundwater aquifer zone, are output to files with the following association (INTERA, 1983c, pp. 51-53):

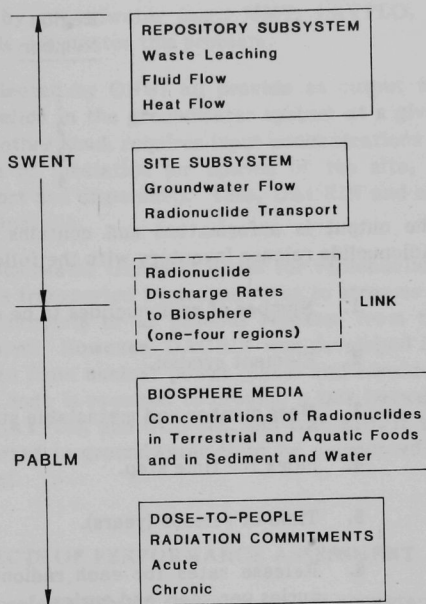


FIGURE 3 Block Diagram Showing Processes Covered by SWENT and PABLM, and Information Covered in SWENT-PABLM Link

<u>Region Number</u>	<u>Tape Unit Number</u>
1	41
2	42
3	43
4	44

The output is unformatted and contains radionuclide discharge data tabulated as a radionuclide release inventory with the following information:

1. Number of radionuclides to be evaluated (maximum 100).
2. Element symbol.
3. Mass number and metastable state.
4. Index for time step.
5. Time of release (years).
6. Release rates for each radionuclide in curies per square meter, curies per year, and curies.

An example of SWENT output can be found in the PABLM input file for the sample PABLM problem given in INTERA (1983d, pp. 75-77).

Although SWENT establishes four intermediate data files corresponding to the four regions, PABLM only processes one region for each computer run. Thus, four runs of PABLM are required to process dosage information for four SWENT regions. Because the PABLM code reads the radionuclide release inventory only from tape unit 41 or an input card deck, the four region tapes (41, 42, 43, and 44) have to be renamed "41" for SWENT-generated data (see Fig. 4).

2.3.3 Conceptual and Operational Links between Models

While the links between some models may be conceptually apparent, they are found upon close examination to be tenuous in an operational sense. The link between a

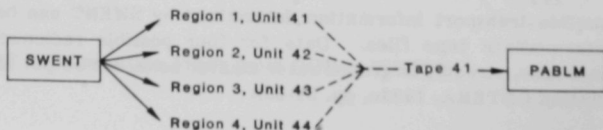


FIGURE 4 SWENT-PABLM Link for Four Hypothetical Radionuclide Discharge Regions

code that addresses radionuclide transport by groundwater (e.g., MMT, LAYFLO, or UCB-NE) and DACRIN, an inhalation dose code, illustrates this problem.

The groundwater transport codes selected by ONWI all provide as output the concentration or flux of a particular radionuclide in the groundwater system at a given distance from a repository. DACRIN, on the other hand, requires input concentrations of radionuclides in the atmosphere at the site of inhalation (or upwind of the site, as DACRIN can account for atmospheric transport and dispersion). Thus, DACRIN and any of the groundwater codes are not directly compatible.

The conceptual link between the groundwater transport codes for radionuclides and DACRIN does exist; that is, radionuclides transported by groundwater to streams or surface outcrops could become airborne in droplets or as gaseous releases from the water, travel in the atmosphere, and be inhaled. However, DACRIN was developed for evaluating inhalation of radionuclides released from nuclear power plants and considers only initially airborne sources. Thus, a new code is required to provide a link between groundwater transport codes, such as MMT, LAYFLO, and UCB-NE, and DACRIN, if the inhalation threat from radionuclides transported in groundwater is to be considered in postclosure repository performance assessment.

2.4 VERIFICATION AND VALIDATION ASPECTS OF PERFORMANCE ASSESSMENT

There are two important aspects of performance assessment: one is acceptance of repository performance by DOE and its contractors, which are examining performance in detail for many designs and scenarios, and the other is acceptance of performance by the technical community external to the detailed process, including NRC, which will have a more limited view of the assessment process. Verification and validation of assessment technologies (model codes) are critical aspects of acceptance by both groups. However, they are particularly important to the external technical community which, for the most part, will view only the tools of assessment (codes) and selected results of code application. Careful and thorough documentation of model construction, performance, and verification and validation histories is the essential ingredient for communication with the external technical community. The communication needs to be clear enough to foster understanding and appreciation of the work, at the very least, and should facilitate external use of the codes, where possible. Because "verification" and "validation" can be ambiguous terms, they require consistent and clear application during performance assessment for the results of such assessments to have a favorable impact on the external technical community.

The external technical modeling community requires that model performance be discussed not only in terms of computed numbers but also in terms of the physical, chemical, and biological processes being simulated. Thus, documentation of code performance should include discussions of model capabilities and results that focus on processes. For example, model response studies will be conducted to demonstrate that model predictions are appropriate for limiting cases where specific results (analytical solutions) or general process behavior is known. If codes for groundwater transport of radionuclides are configured to handle hydrodynamic dispersion, then the codes will be exercised with and without dispersion to determine whether general dispersive features

are present. Similar demonstrations will be made for sorption effects and radioactive decay. Basic model response studies are, of course, only the beginning of model performance assessment, but they provide the foundation for acceptance and should be documented.

Few models are ever verified or validated in a global, or universal, sense; that is, certified verified or valid over the entire range of parameters and for all conceivable applications. Most models are verified or validated in a local sense; that is, over a limited range of parameters for a limited number of applications (House, 1974; Mankin et al., 1977; Shaeffer, 1980). Therefore, statements of verification or validation need to be specific; that is, constrained by the particular conditions under which each exercise was conducted. Otherwise, "verified" and "validated" codes will be applied, with mistaken confidence, in situations where their performance may be in doubt. This problem can be particularly acute in the case of sophisticated, multidimensional, multiprocess models that have, in principle, the capability of being used for a wide range of parameters and combinations of parameters. Model testing that is limited to a few of the possible combinations of parameters does not provide a convincing case for assessment of code performance. Consequently, a carefully planned series of tests over several important combinations of conditions may be required for a credible assessment. Documentation of the results of such tests must be specific with regard to the code capabilities actually tested.

In the case of verification (assuring that the computer code correctly performs those operations specified in the underlying mathematical model), the opportunities to conduct exercises over a pertinent range of conditions may be greater than for validation because verification does not depend on real data sets. Analytical solutions for idealized geometries and simplified processes are the obvious starting points for verification tests, along with the standard exercises of varying the magnitudes of important terms, interchanging axes, and the like. Comparing the results from several codes applied to common problems, such as those developed in the INTRACON meetings (Jansen and Hewitt, 1982), constitutes a clearly valuable verification test as well.

Verification exercises need to be focused on problems inherent to code operation for nuclear waste storage in salt. For example, accumulation of numerical errors may remain at acceptable levels for short-term transient or steady state conditions presumed for a particular analytical solution, while application of the code for repository purposes may require calculations over long periods over which such numerical errors may grow large. Related questions concerning the maximum size of a time step that can be employed while maintaining stability may arise outside of conventional or test cases available from existing nonrepository studies using the code. In summary, verification exercises should be reported in specific terms. The ranges of parameter variations, the dominant processes operable in the test, and the code responses to variations in parameters characterizing the numerical scheme used should be covered.

In the case of validation of a model code (assuring that the code correctly represents the process or system it simulates), fewer opportunities to test code performance over a wide range of conditions are usually available than for code verification. Because validation requires sets of data based on real processes, the data available for validating a code are usually limited. In the case of nuclear waste storage,

some data will be impossible to obtain. Hence, global validity of a code is almost impossible to achieve. Validity consistency is often sought by validating ranges of code behavior against different and independent sets of data. As in the case of verification, care must be taken to note the relationship between the conditions obtaining in validation data sets and those likely to obtain in waste storage applications. The length of the time scales may be the most obvious difference in many cases.

Validation exercises for codes or data sets developed for nuclear power plant licensing may not be directly applicable to waste storage problems. Groundwater flow models "validated" for porous media, where dissolution was slow, may have little meaning in salt formations, and new validations will have to be carried out. As in the case of verification, conducting credible validation exercises requires not only careful selection of exercise parameters but also detailed reporting of validation results in terms of the specific ranges of parameters considered and the relationship of the ranges to anticipated repository problems.

Whenever code results are verified by comparison with analytical solutions or with results from other codes, the issue arises as to how to characterize the comparisons. Statements such as "the agreement was very good" or "the results are close" quickly lose meaning for all but the simplest cases. Plots of the output of single-variable models against other model results provide easily visualized comparisons. But, as the number of code dimensions and variables increases and transient solutions are sought, such displays are no longer simple. Also, an isolated view of a single parameter at a single point in a three-dimensional field as the parameter changes in time may provide a distorted picture of model performance throughout the entire field. Thus, lumped or aggregated quantities may provide a more useful basis for comparison.

The same is true in validation studies when model results are compared with data. Measures of deviation between results and data can be devised for single parameters, while lumped or aggregated deviations can provide quantitative measures that span spatial or temporal fields. Fourier norms of predictions and data, comparisons of cumulative vector averages, and power spectral density estimate comparisons can illuminate gross model performance (Allender, 1976). Statistical measures, including t-tests, correlations, and regression, can be applied in some cases to quantitatively measure model performance (Thomann, 1980). While it is unlikely that any one or group of such techniques for quantifying agreement will provide a totally satisfactory means of assessing the degree of verification or validation, the techniques greatly enhance evaluations of model performance. Moreover, the objective nature of carefully specified quantitative measures of model performance allows clearer and more convincing communication of assessment results to the outside technical community than the subjective "good," "fair," or "poor" designations often used.

2.5 REFERENCES FOR SECTION 2

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INTERA Environmental Consultants, Inc., *VISCOT: A Two-Dimensional and Axisymmetric Nonlinear Transient Thermoviscoelastic and Thermoviscoplastic Finite-Element Code for Modeling Time-Dependent Viscous Mechanical Behavior of a Rock Mass*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-437 (1983b).

INTERA Environmental Consultants, Inc., *A Three-Dimensional Finite-Difference Code for the Simulation of Fluid, Energy, and Solute Radionuclide Transport*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-457 (April 1983c).

INTERA Environmental Consultants, Inc., *PABLM: A Computer Program to Calculate Accumulated Radiation Doses from Radionuclides Transported to Aquatic and Terrestrial Pathways in the Biosphere*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-446 (1983d).

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3 CODE STATUS SUMMARIES

The following summaries of model codes that are candidates for performance assessment application focus on three main areas: (1) purpose, capabilities, and limitations of the codes; (2) status of the elements of documentation and review essential for code verification and validation; and (3) proposed application of the model for performance assessment of salt repository systems. The status of verification and validation activities has been reported in terms of presently available documented reports, not in terms of future plans. Particular attention has been paid to the results of verification and validation activities as far as their impact on the application of the model to the specific problems of waste disposal in salt. Also included in the summaries are discussions of the important relationships among different codes and, in some cases, critiques of the existing documentation for each code and evaluations of code performance.

Areas covered in each model code summary are:

1. Code Name. An acronym has been assigned by ONWI for the performance assessment function.
2. Code Description. A general description of the purpose and methods of approach of the model is given in terms of what the model provides for given inputs. Assumptions about the governing processes are outlined, and the method of calculation or solution is discussed. Limitations of both the approach and solution technique are indicated. Computing machine and software requirements are included.
3. Development Stage. Stage of model development refers to distinctions between recently coded models and well-established models in later versions. References to the original or antecedent models and codes are provided.
4. Documentation. The primary measure of adequacy of documentation is NUREG-0856 (Silling, 1983).^{*} The specific guidelines for document content, not just format, have been compared with available model code documentation. Exceptions to NUREG-0856 guidance and important gaps in documentation are noted.
5. Performance Specification Review. The performance specification review includes examination of the conceptual design of the model, an analysis of its scope, the adequacy of the mathematical model and derivations, the range of model applicability, and the

^{*}Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Comm. Report NUREG-0856 (1983).

input/output requirements. While developers of model codes often address such issues, performance specification review in the code summaries focuses on external review of these items, independent of any reviews that may have been conducted by model code developers and independent of the context of nuclear waste storage in a salt environment.

6. Code Design Review. Code design review includes examination of equations of the numerical model, numerical solution technique, computational error and solution stability, system interfaces, and input/output structures. The summary focuses on external, independent reviews of these items within the context of radioactive waste isolation in salt.
7. Verification. Verification studies are tests and evaluations conducted to assure that a computer code correctly performs the operations specified in a mathematical model. As such studies rarely cover the entire range of possible applications of a model code, the summary specifically identifies those verification studies that have been conducted and the results. This approach informs the reader of the extent to which the code has been exercised. Such exercises will certainly aid in the planning of additional testing and in potential applications.
8. Validation. Validation studies are tests and evaluations conducted to assure that a model as embodied in a computer code is a correct representation of the process or system being modeled. As in the case of verification, the summary seeks to identify and distinguish among various existing validation studies. Such studies will assist in planning model applications and in evaluating suitability.
9. Proposed ONWI Application. On the basis of ONWI documents, the proposed use of the model code is noted. The types of performance assessment (waste package, repository, and site) for which application is planned are identified, as well as the particular problems addressed by the code. The use of similar codes for the same applications may be noted as well, with discussions of the distinctions among the codes.
10. Relationship of Model to Other Codes. The primary issue addressed here is whether the code stands alone or requires input from other codes. Links to other codes in terms of output of the subject code are also indicated. Constraints on input and output data resulting from such linkages are noted.
11. Application of Code to Other Problems. Documented applications of the code to nonsalt or nonrepository situations are listed here.

The relevance of these applications to that of radioactive waste isolation in salt is discussed.

12. Suitability of Model for Salt Repository Application. Limitations of the model that may make it unsuitable for performance assessment of repositories in salt are given. Uncertainties about the applicability of the model to salt as an isolating medium are also raised.
13. Peer Review. Documented independent peer reviews of model code specifications, design, or performance by recognized expert peer groups are cited.
14. References. The references cited are listed at the end of each summary.

3.1 CFEST: A MULTIDIMENSIONAL FINITE-ELEMENT CODE FOR ANALYSIS OF COUPLED FLUID, ENERGY, AND SOLUTE TRANSPORT

3.1.1 Code Description

CFEST (Gupta et al., 1982, PNL-4260) is a coupled fluid, energy, and solute transport code that simulates seasonal energy storage in underground confined aquifers in three dimensions. It treats single-phase Darcy flows in a horizontal or vertical plane, or in fully three dimensional space under isothermally variable conditions. The special case of axial symmetry in a vertical cross section can also be treated. Both steady state and transient simulations are possible. The code is designed to operate in an interactive mode to aid in understanding complex aquifer systems. It can also be used to help design field experiments and to interpret sparse field data.

Input requirements include fluid and hydrogeologic properties, which can be dependent on or independent of head, temperature, solute concentration, and fluid density. Fluid properties include compressibility, thermal coefficient of expansion, solute concentration (only one species is allowed), heat capacity, internal energy, and viscosity. Overall aspects of the geologic region and the constituent geologic units must be specified. The isotropic or anisotropic properties of each confining rock unit that must be entered include permeability, porosity, compressibility, specific storage, dispersivity length, thermal conductivity, heat capacity, and thermal properties.

The model is based on three governing partial differential equations, namely, conservation of total liquid mass, conservation of energy, and conservation of mass of dissolved contaminant. They are coupled through fluid density, which is expressed as a function of pressure head, temperature, and solute concentration. These three dependent variables are functions of space and time. Fluid viscosity is a function of temperature and solute concentration. Flow is transient and laminar (Darcian). Aquifer properties (porosity, permeability, and thickness) may be space-dependent. Hydrodynamic

dispersion is a function of fluid velocity. Boundary conditions permit heat losses or gains to adjacent formations, natural movement of water in the aquifer, and arbitrary location of wells. The fluid and the porous media are compressible, whereas rock density and heat capacity are treated as constants. The energy balance ignores viscous dissipation.

The code employs a staged execution structure and can be operated in an interactive mode. It uses a right-hand Cartesian coordinate system throughout. The two- or three-dimensional modeled domain is assumed to be bounded by piecewise smooth boundaries. In addition to the three basic conservation equations, the model also specifies fluid density and porosity relations. Density is expressed as a function of the solute concentration, temperature, and pressure head using only the zeroth- and first-order terms of a Taylor series. Porosity is expressed in terms of compressibility. These relations are substituted into the three basic conservation equations, which are then solved using the Galerkin finite-element method. Gaussian quadrature is used to integrate the finite-element equations numerically. The following processes are not considered: adsorption into a porous media substrate, chemical reactions in solution, and radioactive decay chains.

Source language and machine requirements are not mentioned in PNL-4260.

3.1.2 Development Stage

CFEST is a fully operational code that is an extension of the finite-element three-dimensional groundwater code (FE3DGW) developed by Gupta et al. (1979). CFEST has been technically documented and tested, but no user's manual is available.

3.1.3 Documentation

Current documentation is limited to PNL-4260, which is not intended to be a user's manual. Hence, it does not conform to NUREG-0856 (Silling, 1983). Another major omission from PNL-4260 is a software summary that provides information about source code language and machine requirements. Also, no information on code custodianship or responsibility for revisions and updates is given. A code listing was not included. Aside from these deficiencies, model theory and methods of solution are adequately treated, as is verification.

3.1.4 Performance Specification Review

No internal or external performance specification review is documented.

3.1.5 Code Design Review

No internal or external code design review is documented.

3.1.6 Verification

Several tests conducted by the code authors to check the correctness of the coding and to test the sensitivity of the results to grid and time-step size are discussed in PNL-4260. Results of these tests are summarized below.

1. Steady drawdown from flow to a well in a confined aquifer. CFEST results were compared with published analytical results that assumed axial symmetry. Results showed excellent agreement for a fine, axisymmetric grid system. Results were slightly sensitive to choice of grid (i.e., Cartesian versus cylindrical coordinates) and grid spacing.
2. Unsteady drawdown from flow to a well pumped at a constant rate in a vertically confined but horizontally infinite and isotropic aquifer. CFEST results were compared with published analytical results that assumed axial symmetry. Results showed excellent agreement for long time periods but somewhat poorer agreement for short time periods.
3. Unsteady drawdown from flow to a steadily pumped well draining an elastic artesian aquifer confined by semipervious (leaky), elastic strata. The flow is vertical through the confining formations and horizontal through the aquifer. The flow region is occupied by five layers. CFEST results were compared with published analytical results. Results showed good agreement for several radii and all except the shortest dimensionless times.
4. Uniform regional flow with sources and sinks. CFEST results were compared with published analytical results. Results on a two-dimensional plane showed good agreement, with accuracy somewhat dependent on grid structure.
5. Dirichlet upstream boundary condition test; linear, one-dimensional geometry. CFEST results were compared with published results, with good agreement.
6. Mixed upstream boundary condition test, one-dimensional geometry. CFEST results were compared with published results. Results showed good agreement, with absolute errors somewhat dependent on time-step size.
7. Single well problem, with radially varying velocity and dispersion. CFEST results were compared with an approximate analytical solution. This is the first test with variable velocity and dispersion. Results compared reasonably well; discrepancies were attributed to the approximate nature of the analytical solution.

8. Energy transport including cap and bedrock conduction. This is the first test involving energy loss to the confining media. CFEST results were compared with two published analytical solutions. Results verified CFEST's capability to simulate conductive heat loss in conductive cap rock and bedrock.

3.1.7 Validation

No validation of CFEST has yet been reported. PNL-4260 indicates that validation tests are planned in connection with Battelle Pacific Northwest Laboratories' seasonal thermal storage program.

3.1.8 Proposed ONWI Application

CFEST, along with DOT, HEATING6, and SWENT, are listed by ONWI as potentially useful in analyzing waste package thermal boundaries. It is similarly listed as suitable for temperature analyses within the waste package for repository subsystem thermal environment and fluid assessment, and for groundwater flow and hydrologic budget analyses.

These applications all require CFEST's multidimensional flow and energy transport simulation capabilities. The inputs required for such simulations include specification of the various geologic units making up the flow system as well as various fluid and media properties.

3.1.9 Relationship of Model to Other Codes

CFEST is a stand-alone, general-purpose model that simulates complex aquifers. However, for application to salt repository problems, detailed properties of solutions (including concentrations of radionuclides and other species), geologic aquifers, and confining strata would be required as a function of time. Because chemical reactions, adsorption, radioactive decay and formation, and flow through fractured media are not treated, CFEST would have to be operated in tandem with codes having such capabilities. Because none of the codes presently cited by ONWI possess all of these capabilities, several would have to be operated in an iterative mode. For example, while geochemical codes can provide input on solution speciation, phase distributions, and radionuclide abundances (PHREEQE and EQ3/EQ6), other codes will be required for flow in deformed media (STAFAN) or through fractured media (FTRANS). In the vicinity of the waste package or within it, source codes like WAPPA will be required to provide input data on leachates and thermal conditions.

3.1.10 Suitability of Model for Salt Repository Application

The suitability of the model for salt repository applications has not been addressed in ONWI documents or in PNL-4260. CFEST was developed at Pacific

Northwest Laboratories for use in its seasonal thermal storage program and was never considered by the authors for use in a salt repository environment. For far-field or regional applications outside of the salt deposit, CFEST appears to be well suited to the problem of transport of contaminated groundwater through a complex of unfractured geological formations, provided that chemical reactions, adsorption, and radioactive decay and formation are not important. Because of its ability to treat rather general formations, it could be used for analyses supplemented by other codes that treat these other aspects in detail but place less emphasis on the hydrological aspects of the problem. The same may be said for the waste package environment after resaturation of the salt deposit and backfill has occurred. However, applicable ranges of temperature and pressure are not documented.

3.1.11 Peer Review

Any peer review should address the role that CFEST could play in salt repository performance assessment. No documentation on peer reviews is available.

3.1.12 References for Section 3.1

Gupta, S.K., et al., *A Multidimensional Finite-Element Code for the Analysis of Coupled Fluid, Energy, and Solute Transport (CFEST)*, Battelle Pacific Northwest Laboratories, Richland, Wash., PNL-4260 (Aug. 1982).

Gupta, S.K., et al., *Methodology for Release Consequences Analysis, Part III: Finite-Element Three-Dimensional Ground-Water (FE3DWG) Flow Model*, Battelle Pacific Northwest Laboratories, Richland, Wash., PNL-2939 (Sept. 1979).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

3.2 DACRIN: A COMPUTER PROGRAM FOR CALCULATING ORGAN DOSE FROM ACUTE OR CHRONIC INHALATION OF RADIONUCLIDES

3.2.1 Code Description

DACRIN (INTERA, 1983, ONWI-431) rapidly calculates consistent estimates of the effective radiation dose to the human respiratory tract and other organs, resulting from inhalation of radioactive aerosols. The code is an outgrowth of the development of a mathematical model for organ dose that follows the basic precepts of the International Commission on Radiological Protection (ICRP) task group on lung dynamics (ICRP, 1959). Mathematical models describing atmospheric dispersion have also been included as part of the code's evaluation of doses resulting from either accidental or chronic atmospheric releases of radionuclides.

For each case, the code calculates the effective radiation dose to any of 18 organs and tissues from inhalation of any one or a combination of no more than 10 of the over 600 radionuclides considered by ICRP. Organ doses are calculated by specifying either the quantity of radionuclide inhaled or the quantity released to the atmosphere. In the latter case, duration of release, release height, wind speed, atmospheric dispersion parameters, and downwind distance at which the dose is to be calculated must also be specified. As many as 10 distances may be specified for each use.

Required input consists of a few program control variables, the duration of inhalation exposure, the ventilation rate, the time interval within which the dose is delivered, the organs of interest, the quantity of radionuclide inhaled, its solubility class and particle size, and, when an atmospheric dispersion model is involved, the additional parameters required for the model selected. Output consists of the effective radiation doses to the specified organs at selected time intervals for each radionuclide inhaled.

DACRIN is based on the precepts of the ICRP task group on lung dynamics and a simple exponential model for retention by an organ of interest. The model divides the respiratory tract into three regions: nasopharyngeal, tracheobronchial, and pulmonary. Deposition is assumed to vary with the aerodynamic properties of the aerosol distribution. Atmospheric dispersion is described by a bivariate normal distribution model incorporated into the code; however, normalized air concentrations at specific distances as calculated by any other atmospheric dispersion model can be used as input. All atmospheric dispersion and dose equations are directly dependent on the values of input parameters and are solved analytically. There may be no more than 10 downwind distances at which dose is calculated, 10 organs of interest, 10 time intervals measured from the most recent intake, and 5 multiple intake intervals.

The complexity of the model, or programming class, is designated in Science Applications (1981) as B/C, indicating a program of 250-1000 lines of instruction that requires a minimum configuration of a minicomputer to a super minicomputer, with an approximate setup time of 30 minutes to one hour and an approximate execution time of two hours. The programming language is FORTRAN (FORTRAN V for the SCEPTER version of DACRIN), and the computers for which the program is designed are the UNIVAC 1100 and CDC CYBER 176. Fifty-six thousand words of memory are needed to execute the code. Compiling the DACRIN source and executing a sample problem required 100 seconds of central processing unit (CPU) time on a UNIVAC 1100/44.

3.2.2 Development Stage

CDC and UNIVAC versions of DACRIN are available and operational (National Energy Software Center, 1981; Science Applications, 1981). DACRIN was originally developed for use on UNIVAC machines by Battelle Pacific Northwest Laboratories (Houston et al., 1977). It was adapted for CDC machines and modified and revised in ONWI-431, in order to include it in the SCEPTER project. The changes made include (1) conversion for use with a CDC computer, (2) removal of defunct print options, and (3) insertion of a unique code identification number that must be matched to allow execution.

3.2.3 Documentation

The CDC version is documented in ONWI-431 in accordance with NUREG-0856 (Silling, 1983), including the federal information processing standard software summary, user's manual, and other required features. The UNIVAC version is fully documented in Houston et al. (1977) and further documented in National Energy Software Center (1981). Additional documentation, including summary documentation, is available in Streng (1975), Miller (1978), Shriner and Peck (1978), and Science Applications (1981).

3.2.4 Performance Specification Review

The UNIVAC version has been accepted by the nuclear industry and NRC, and has been used extensively in the licensing of nuclear projects (U.S. Department of Energy, 1980; Office of Nuclear Waste Isolation, 1983a). No documented additional review has been performed for performance assessment purposes.

3.2.5 Code Design Review

The UNIVAC version has been accepted by the nuclear industry and NRC, and has been used extensively in the licensing of nuclear projects (U.S. Department of Energy, 1980; Office of Nuclear Waste Isolation, 1983a). No additional documented review has been performed for performance assessment purposes.

3.2.6 Verification

Verification tests have been conducted on the original DACRIN code (Houston et al., 1977) and the DACRIN code as modified for the SCEPTER project (INTERA, 1983). The same two sample problems were run in each case.

Verification problem 1 demonstrated the chronic dose calculation. It used the direct inhalation option and consisted of a calculation of the dose to 10 different organs or tissues from chronic inhalation of a mixture of fission products for five dose times following termination of uptake.

Verification problem 2 was an acute dose problem. It made use of the atmospheric diffusion model built into the program that uses the Simpson-Fuquay stable atmospheric diffusion model option to calculate the dose to four organs at two dose times following passage of a cloud produced by short-term release to the atmosphere of a mixture of transuranic nuclides.

Calculated dose results for these two problems using both the modified-for-SCEPTER and unmodified DACRIN codes are reported to have matched exactly when identical organ data libraries were used (INTERA, 1983).

3.2.7 Validation

Although DACRIN is based on the respiratory tract model adopted by the ICRP task group on lung dynamics (ICRP, 1959) and has been applied to nuclear-waste-isolation-type situations, no formal validation of the model has yet been documented. Office of Nuclear Waste Isolation (1983b) states on page 133 that codes reflecting ICRP-30 methodology should be used. Because DACRIN is based on an ICRP-2 model, this discrepancy should be justified.

3.2.8 Proposed ONWI Application

DACRIN will be used for environmental radiological exposures under normal operation of a nuclear waste repository in salt and also for environmental radiological exposures from repository accidents.

Because DACRIN calculates atmospheric dispersion and radiological doses via inhalation, it is appropriate for analyzing scenarios in which radioactive wastes are transported from the repository system into the atmosphere. Envisioned events that may allow for such transport include drilling into or mining of the waste or waste package, magmatic or volcanic events that would bring waste to the surface, transport of aerosols associated with contaminated irrigation water, and windblown erosion of contaminated soils.

DACRIN does not estimate the releases that would occur in situations such as those mentioned above. These releases must be estimated by other codes and supplied as input to DACRIN. Such input might include the likelihood and degree of geologic or human intrusion events, waste composition, waste release concentrations, waste particle sizes, meteorological conditions, and human population information, such as population distribution and cultural practices that could affect inhalation exposure.

Once such information is provided, DACRIN can be used to evaluate, in part, the impacts of radionuclide releases in terms of dose to particular organs or tissues. DACRIN does not estimate the dose associated with ingestion or external exposure; this information can be obtained from PABLM. These two dose assessment codes can then be used to determine the relative importance of radionuclide releases, thereby providing more complete assessments of repository systems.

In salt repository assessments, DACRIN can be most useful for safety calculations associated with the operational phase. However, certain special scenarios associated with assessment of long-term isolation performance may require the capabilities of this code. Examples of long-term scenarios that could result in atmospheric releases are direct drilling through a canister or solution mining accompanied by surface storage of insolubles.

An example of a salt repository problem for which an acute dose calculation using DACRIN would be appropriate would be a situation in which a waste canister is ruptured, resulting in the sudden release of material in the presence of humans. A chronic dose calculation using DACRIN would be appropriate if nuclear waste material

were inadvertently brought to the surface by mining or some other method and allowed to remain exposed to the elements for a period of time in the vicinity of humans.

3.2.9 Relationship of Model to Other Codes

Many other biosphere transport and radiological dose codes exist; a tabulation of a subset of these codes used in nuclear waste isolation applications is found in Science Applications (1981). Other programs that calculate organ dose include SUBDOSA, which calculates external doses from atmospheric releases of radionuclides; AERIN, which calculates organ and tissue burdens resulting from acute exposure to a radioactive aerosol; and ARRRG, FOOD, and PABLM, which calculate radiation doses to humans from radionuclides in the environment. The two data libraries used by DACRIN are RMDLIB, the radionuclide decay data library, and ORGLIB, the organ data library.

More than one version of DACRIN is extant. The version documented in ONWI-431 incorporates the minor changes made to provide consistency with the SCEPTEr technology package (Brecher and Pearson, 1983; INTERA, 1983).

3.2.10 Application of Code to Other Problems

This code has been extensively used in the licensing of nuclear projects.

3.2.11 Suitability of Model for Salt Repository Application

Because the dosimetry model is independent of the origin of the radionuclides, DACRIN is applicable to salt repositories. Also, there are no unique aspects to its application to a nuclear waste repository in salt.

3.2.12 Peer Review

ONWI has no plans for peer review (Office of Nuclear Waste Isolation, 1983a).

3.2.13 References for Section 3.2

Brecher, A., and F.J. Pearson, Jr., *The SCEPTEr Waste Package Subsystem Computer Model for Performance Assessment*, in Scientific Basis for Nuclear Waste Management VI, D.G. Brookins, ed., North-Holland Publishing Co., New York, N.Y. (1983).

Houston, J.R., et al., *DACRIN — A Computer Program for Calculating Organ Dose from Acute or Chronic Radionuclide Inhalation*, Battelle Pacific Northwest Laboratories, Richland, Wash., BNWL-B-389 (Dec. 1974, reissued April 1976, and errata published Dec. 1977).

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Shriner, C.R., and L.J. Peck, *Inventory of Data Bases, Graphics Packages, and Models in Department of Energy Laboratories*, Oak Ridge National Laboratory Report ORNL/EIS-144 (Nov. 1978).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

Streng, D.L., *DACRIN — A Computer Program for Computing Organ Dose from Acute or Chronic Radionuclide Inhalation: Modification of Gastrointestinal Tract Dose*, Battelle Pacific Northwest Laboratories, Richland, Wash., BNWL-B-389 SUPP (Feb. 1975).

U.S. Department of Energy, *Final Environmental Impact Statement — Management of Commercially Generated Radioactive Waste*, DOE/EIS-0046 F (Oct. 1980).

3.3 DOT: A NONLINEAR HEAT-TRANSFER CODE FOR ANALYSIS OF TWO-DIMENSIONAL PLANAR AND AXISYMMETRIC REPRESENTATIONS OF STRUCTURES

3.3.1 Code Description

The DOT code (INTERA, 1983, ONWI-420) predicts temperature as a function of time and position for two-dimensional planar or axially symmetric systems. Input consists of (1) system geometry; (2) material properties (thermal conductivity, heat capacity, and mass density); (3) initial and boundary conditions; and (4) internal heat generation rate per unit volume as a function of time and position. Thermal conductivity and heat capacity are specified as functions of position and temperature, whereas mass density is specified as a function of position only. Thermal conductivity can be anisotropic or isotropic. The code solves the partial differential equation for time- and space-dependent heat flow using a finite-element method. Aside from the restriction to two dimensions, limitations of the code include the assumptions that heat transfer is only by conduction, and not by radiation or convection, and that no phase changes occur in the pore fluid. A further limitation is the requirement for a constant time step with each execution of the program.

The DOT code is written in FORTRAN IV for use on a CDC CYBER 176 computer.

3.3.2 Development Stage

The DOT code is complete and available for use.

3.3.3 Documentation

The documentation of DOT in ONWI-420 is quite good and follows the NUREG-0856 guidelines (Silling, 1983). It could be improved, however, by making the following relatively minor changes:

1. Replace "Q = heat generation rate" by "Q = heat generation rate per unit volume" (p. 2).*
2. Replace "C = specific heat capacity" by "C = specific heat capacity per unit mass" (p. 2).
3. Insert a statement pointing out that while q_n is the heat flow in the direction of n , $\partial T / \partial n$ is evaluated in the direction opposite to n (p. 3). (Here, n is the outward normal to the surface.)

*Page numbers in Sec. 3.3 are from ONWI-420.

4. Point out that N must be an odd integer (p. 3).
5. Replace " $\partial T / \partial n$ " by " $\partial T / \partial x_i$ " (p. 19).
6. Insert a brief section in, say, Sec. 3 that discusses the applicability of the model to a geologic repository. The comments in Sec. 1.2 are too brief and too general.
7. Section 4 (Verification Tests and Results) should be expanded along the lines indicated in Sec. 3.3.6.
8. The symbol V should not be used for both "radiation view factor" and "volume" (pp. 10 and 19).
9. "Radiation view factor" should be explicitly defined (p. 10).

3.3.4 Performance Specification Review

Performance specification review is not known to have been completed.

3.3.5 Code Design Review

Code design review is not known to have been completed.

3.3.6 Verification

Two types of verification tests have been applied to the DOT code: (1) comparison of the DOT solution to various problems with the analytical solutions to the same problems and (2) comparison of the DOT solution to various problems with the solutions to the same problems generated by independent codes. These tests and the test results are summarized in Table 2.

The following conclusions can be drawn from the test results given in Table 2.

1. No major or systematic errors were found in the DOT code.
2. Good to excellent agreement was obtained for all tests, with the exception of one spatial point in the second test of type 2. In this case, the code with which DOT was compared might be inaccurate.
3. In the third type-1 test, the discrepancy was increasing with time. Could this increase be reduced by reducing the size of the time step? What is the reason for the increase?
4. The DOT code appears to be quite accurate over the range of parameters tested.

TABLE 2 Verification Tests Applied to DOT

Test Type	Test	Result
1	Steady state heat conduction in a square plate	Excellent agreement (i.e., essentially no discrepancy on visual inspection of the comparison plot)
1	Steady state heat conduction in a long, hollow cylinder	Excellent agreement
1	Internal heat generation in a parallel-sided slab	The discrepancy between the two solutions is less than or equal to 2% from t (time) = 0 out to $t = 0.32$ seconds, but is increasing with time. (What is the cause of this discrepancy and will it continue to increase with t ?)
1	Transient heat conduction in a semi-infinite solid subjected to a unit surface heat flux	Excellent agreement in the case of the temperature versus depth plot; discrepancies of 0-4% in the case of the surface temperature versus time plot
1	Transient heat conduction in a finite length rod	Agreement within approximately 1%
1	Transient heat conduction in an infinite parallel-sided slab	Excellent agreement
2	Nonlinear transient heat conduction through an infinite parallel-sided slab	Agreement within 1%
2	Nonlinear transient heat conduction in a square concrete column uniformly exposed to an American Society for Testing and Materials fire	Close agreement at two spatial points, but only within approximately 10% at a third. (The reason for this difference is not clear.)

While the eight verification problems test many of DOT's capabilities, not one of them tests DOT's capability for simulating systems having anisotropic thermal conductivity. Also, the tables of input data in ONWI-420 (e.g., the table in Sec. 4.2.1) need to be better explained. In their present formulation, the tables convey almost no useful information. Finally, the information provided in the description of the first verification test is insufficient to allow repetition of the test.

3.3.7 Validation

The DOT code has been used to predict temperatures in underground heating experiments conducted in granite at Stripa, Sweden. Temperatures predicted by the model were found to agree well with observed temperatures (Chan et al., 1980).

3.3.8 Proposed ONWI Application

The DOT code will be used to predict the temperature distribution within the repository. It could also be used for waste package assessment. Although similar to HEATING6, DOT is limited to two dimensions, whereas HEATING6 can accommodate three. For two-dimensional situations, DOT is generally more applicable than SALT-4. The DOT code can simulate the response of the repository to either a single waste package or an infinitely long array of such packages, while TEMP can simulate repository response to an array of arbitrary length, provided the array is embedded in a volume of constant isotropic thermal conductivity.

3.3.9 Relationship of Model to Other Codes

The temperature field produced by DOT is used as input to the thermomechanical stress analysis codes VISCOT, MATLOC, and UTAH 2.

3.3.10 Application of Code to Other Problems

Chan et al. (1980) report using DOT to predict temperatures in underground granite at Stripa, Sweden.

3.3.11 Suitability of Model for Salt Repository Application

In applying DOT to a repository in salt, the following limitations are encountered:

1. The DOT code is limited in applicability to physical systems that are two-dimensional planar or axially symmetric.
2. The DOT code assumes negligible radiative heat transfer. Because salt is transparent at infrared wavelengths, this assumption might

well be invalid for a salt repository. If it is invalid and provided that the distance over which the temperature varies significantly is much larger than the infrared absorption length, one can define an effective total thermal conductivity. This thermal conductivity term would include both conductive and radiative contributions, and could be used as the effective conductivity in the DOT code in place of thermal conductivity.

3. The DOT code assumes no phase change in the fluid. For example, it assumes that water in the interstices of the salt formation does not vaporize. At sufficiently high temperatures, however, this could happen, with the result that convective heat transport (assumed by the model to be negligible) could suddenly become significant.

3.3.12 Peer Review

The DOT code has not been subjected to peer review.

3.3.13 References for Section 3.3

Chan, T., *Heat Transfer in Underground Heating Experiments in Granite, Stripa, Sweden*, in *Heat Transfer in Nuclear Waste Disposal*, F.A. Kulacki and R.W. Lyzchowski, eds., American Society of Mechanical Engineers Monograph HTD, Vol. II, pp. 1-8 (1980).

INTERA Environmental Consultants, Inc., *DOT: A Nonlinear Heat-Transfer Code for Analysis of Two-Dimensional Planar and Axisymmetric Representations of Structures*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-420 (1983).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

3.4 EQ3/EQ6: A GEOCHEMICAL SPECIATION AND REACTION PATH CODE PACKAGE SUITABLE FOR REPOSITORY PERFORMANCE ASSESSMENT

3.4.1 Code Description

EQ3/EQ6 (Wolery, 1979; Thomas et al., 1982; INTERA, 1983a) is a software package consisting of two separate codes. EQ3 is a geochemical code that computes solution speciation, that is, the distribution of ions, ion complexes, and neutral species in an aqueous solution given user specified reactions, elements, and compounds. EQ6 is a geochemical transport code that simulates reaction paths, that is, the sequence of steps

going from equilibrium state to equilibrium state. It calculates changes in phase equilibrium at each intermediate equilibrium step and determines the mass of each constituent transported from one phase to another. Gas, solution, and solid phases are dealt with.

In contrast to PHREEQE (INTERA, 1983b, ONWI-435), a combined speciation/transport code that calculates only the final state from user-specified initial conditions, EQ6 starts with the solution model calculated by EQ3 and simulates small progressive changes while keeping track of interphase transport in each step as the final state is approached. Hence, EQ3/EQ6 is a more detailed and more powerful simulation tool than PHREEQE, but it does require more core memory and computer time. It is also easier to use than PHREEQE. The reaction path simulation is carried out automatically in a single run without the careful hand operations required for a reaction-path simulation with PHREEQE. Because of its computational power and ability to handle intermediate steps in a reaction-path simulation, EQ3/EQ6 is more suited than PHREEQE to applications in the near-field environment (waste package and waste form). Perturbations from equilibrium resulting in significant interphase transport are more likely to occur there than in the far field.

Although any temperature between 0°C and 300°C can be handled, simulation pressures are limited to either a fixed value of 500 bars or one atmosphere for temperatures between 0°C and 100°C or values along the saturated steam curve for temperatures greater than 100°C.

The input data set required to run EQ3/EQ6 includes equilibrium constants for each reaction described by mass-action equations and for each dissolution/precipitation reaction at specified temperatures. These constants are internally corrected for the specific simulation temperature. The data set also includes coefficients used to compute the activity of water as a function of electrolyte concentration and temperature, and the activities of neutral and ionized species as functions of total ionic strength and temperature. Debye-Hückel constants at various temperatures are also included in the data set and are used to compute the activity coefficients of ionized species. The user can choose from several alternative formulas for computing these coefficients. None of the choices is satisfactory for aqueous solutions with ionic strengths greater than 1 molal.

3.4.2 Development Stage

Because the EQ3 and EQ6 codes are relatively new, they have not been widely used. Most of the work on these codes was done at the Department of Geological Sciences, Northwestern University, with subsequent work done at Lawrence Livermore Laboratory (Thomas et al., 1982). The codes are based on earlier work by Garrels and Mackenzie (1967), Helgeson et al. (1970), Wolery (1979), and others.

3.4.3 Documentation

The code as documented in ONWI-472 generally conforms to NUREG-0856 (Silling, 1983), except that the discussions of the theory and solution methods are relegated to an appendix written by one of the code authors rather than by one of the documentation authors. This appendix gives a concise but good general review of geochemical modeling and associated numerical methods, thus providing the reader with some perspective on EQ3 and EQ6. Because the appendix was poorly reproduced, many of the equations are unreadable. With one exception, the documented versions of the codes are the same as those written by the original code authors. Only the preprocessor EQTL has been modified by INTERA (1983b) to form the new code PQLT, which is used to prepare PHREEQE data for EQ3/EQ6.

3.4.4 Performance Specification Review

With regard to requirements for application to repository performance assessment, ONWI-472 makes the comment that "only PHREEQE and EQ3/EQ6 meet certain of the SCEPTER performance requirements (INTERA, 1982b). The particular qualifying requirements were: (1) incorporation of a general algorithm with aqueous species and solid phase identities set by user input, (2) ability to handle temperature variations, and (3) readily available source code and adequate user manual documentation." No documentation of external performance specifications review is available.

3.4.5 Code Design Review

An internal review conducted by INTERA presumably served as the basis for Sec. 3 of ONWI-472. Comparison of the geochemical codes PHREEQE and EQ3/EQ6 suggests that, while the former is designed for relatively fast operation for scope calculations, the latter is a more powerful, if costlier to run, computational tool and is more suited to near-field waste package assessment problems. EQ3/EQ6 is also designed for easier use.

To solve the system of simultaneous, nonlinear, algebraic mass-balance and mass-action equations in EQ3, an iterative solution method is used. EQ6 employs a variation of the differential equation method of solving a system of nonlinear algebraic equations first used by Helgeson et al. (1970). The present method avoids some of the difficulties of an earlier implementation of Helgeson by correcting the predicted values using a Newton-Raphson method to satisfy the original algebraic equations instead of the difference equations that represent the corresponding differential equations (Wolery, 1979). The total software package includes the main codes EQ3 and EQ6, a set of supporting data files, two utility routines for data-file management, and sample input files for EQ3 and EQ6. It has been written for operation on CDC equipment. Both EQ3 and EQ6 require the IMSL subroutine package. The entire package comprises over 30,000 card images.

No external code design review has been documented.

3.4.6 Verification

EQ3/EQ6, with its own thermodynamic data set and with the data set provided with PHREEQE, has been applied to several test problems for code verification, intercode comparison, and illustrative purposes. Three tests are reported in the verification section of ONWI-472; two others that are basically illustrative in nature are reported in the user's manual as example problems.

1. Speciate Major Ions of Seawater. The purpose of problem 1 was to verify EQ3 coding by comparing computed concentrations of free and complexed ions (combinations of four cations and five anions) with those resulting from hand calculations. This comparison was not an adequate verification of EQ3 because the thermodynamic data sets used for EQ3 and the hand calculations were different. The lack of agreement in the results was probably due to the input data differences.
2. Speciate Full Seawater Analysis. The purpose of problem 2 was to compare EQ3 to PHREEQE and WATEQF/WATEQ2 (Plummer et al., 1976), and to test the sensitivity of the thermodynamic data sets. The effect of entering carbon species via "total inorganic" versus "total alkalinity" was on the order of 5% or less. The effect of the two different thermodynamic data sets (one developed for EQ3 and one for PHREEQE) was 10% or less on minor and major ionic species concentrations but was much larger on mineral saturation indices, indicating that the entered thermodynamic data are a major source of uncertainty for such calculations. Code-to-code differences using as close to the same input data as feasible showed generally smaller differences than those obtained from using different data sets with the same code.
3. Dissolve Microcline in Dilute Hydrochloric Acid. The purpose of problem 3 was to illustrate the reaction-path-simulation and phase-boundary-finding capabilities of EQ3/EQ6, and to compare these with those of PHREEQE. An additional purpose was to compare computed phase boundaries with those obtained from hand calculations. Location of phase boundaries was found to be a sensitive function of the thermodynamic input data set. The data sets that came with EQ3/EQ6 and PHREEQE gave substantially different results. Reaction paths were also found to change substantially when the two data sets were used in the same codes. Code-to-code differences when using the same data sets were quite small.
4. Reduce an Oxygenated-Calcite and Hematite-Saturated Solution by Adding Methane. The purpose of problem 4 was to illustrate how EQ3 and EQ6 are used to simulate reaction paths that include redox reactions and to compare results with those calculated using

PHREEQE. Comparisons were close when using the same input data.

5. Carbonate Aquifer Dedolomitization by Gypsum Solution with Increasing Temperature. The purpose of problem 5 was to illustrate the temperature-changing capabilities of EQ6.

Note that PHREEQE does not treat temperature as a dependent variable. It must be entered as input by the user.

3.4.7 Validation

Although no validation efforts have been reported, some comparisons have been made between observations and calculations for a few of the equations used in EQ3 to calculate activity coefficients. Such comparisons suggest that these calculations are generally a major source of uncertainty and pose great difficulties in the case of strong electrolyte solutions and for solutions containing radionuclide-bearing compounds for which few data are available. The following candidate validation exercises have been tentatively suggested by ONWI.

1. Calculating radionuclide solubilities in site-specific far-field brine groundwaters and comparing the results with laboratory measurements.
2. Predicting the pH of far-field groundwaters in equilibrium with the limestones both in situ and after sampling (outgassing of carbon dioxide with consequent pH change) and comparing the results with field data.
3. Predicting the composition of waste-glass leachate or corrosion solutions and comparing the results with those achieved in the laboratory, assuming that the necessary code capabilities and input data are available at the time.

3.4.8 Proposed ONWI Application

In the near field, EQ3/EQ6 will be used to assess geochemical reactions affecting the waste package barriers and near-field transport. The results will be used as input to corrosion and hydrological mass transport codes. In the far field, the code will be used to assess geochemical reactions affecting radionuclide transport. The results will provide inputs to hydrological mass-transport codes. Information required as input to mass-transport codes includes distribution of radionuclide species in dissolved and solid phases as a function of temperature, pressure, and solution composition. To provide such information, the geochemical codes must be able to handle concentrated brine solutions and must have input data on solution reactions involving radionuclide-bearing compounds. Such requirements are difficult to satisfy. Neither PHREEQE nor EQ3/EQ6 possesses the necessary algorithms or input data sets required.

3.4.9 Relationship of Model to Other Codes

To perform calculations within the framework of repository assessment, the model will have to be operated in conjunction with codes that provide information about thermodynamic variables and chemical constituents. It is not clear from the documentation precisely how the various interrelated codes will be operated. In the near field, WAPPA and ORIGEN2 can provide information on rates of heat generation and radionuclide inventories, but neither provides detailed information on the chemical compounds likely to be the constituents of the invading brine solutions from the repository. EQ3/EQ6 can provide input to WAPPA for computing leaching and corrosion. The code can also be used to provide concentrations of radionuclide-bearing compounds to mass-transport codes like SWENT.

3.4.10 Application of Code to Other Problems

Applications to several problems are discussed in Wolery (1979) and Secs. 4 and 13 of INTERA (1983a).

3.4.11 Suitability of Model for Salt Repository Application

For both near- and far-field applications, the code should be able to handle concentrated brine solutions and to predict radionuclide distributions in solution and solid phases as a function of temperature, pressure, and solution composition. Whereas thermodynamic equilibrium is probably acceptable for the far field, it may not be adequate for the near field, where temperature, pressure, and available solid constituents will change as successive waste package barriers are breached. Neither PHREEQE nor EQ3/EQ6 has the required capability for treating brines. Nor is it clear when the necessary thermodynamic data sets will be available.

3.4.12 Peer Review

No documented peer review is available.

3.4.13 References for Section 3.4

Garrels, R.M., and F.T. Mackenzie, *Origin of the Chemical Composition of Some Springs and Lakes*, in *Equilibrium Concepts in Natural Water Systems*, American Chemical Society, Advances in Chemistry Series No. 67, pp. 222-242 (1967).

Helgeson, H.C., et al., *Calculation of Mass Transfer in Geochemical Processes Involving Aqueous Solutions*, *Geochimica et Cosmochimica Acta*, 34:569-592 (1970).

INTERA Environmental Consultants, Inc., *EQ3/EQ6: A Geochemical Speciation and Reaction Path Code Package Suitable for Nuclear Waste Performance Assessment*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-472 (1983a).

INTERA Environmental Consultants, Inc., *PHREEQE: A Geochemical Speciation and Mass Transfer Code Suitable for Nuclear Waste Performance Assessment*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-435 (April 1983b).

Plummer, L.N., et al., *WATEQF: A Fortran IV Version of WATEQ, A Computer Program for Calculating Chemical Equilibrium of Natural Waters*, U.S. Geological Survey Water Resources Investigations 76-13 (1976).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

Thomas, S.D., et al., *A Summary of Repository Siting Models*, prepared for U.S. Nuclear Regulatory Commission by GeoTrans, Inc., NUREG/CR-2782 (July 1982).

Wolery, T.J., *Calculation of Chemical Equilibrium between Aqueous Solution and Minerals: The EQ3/6 Software Package*, Lawrence Livermore Laboratory Report UCRL-52658 (1979). (This report is included as an attachment to ONWI-472.)

3.5 FE3DGW: FINITE-ELEMENT THREE-DIMENSIONAL GROUNDWATER FLOW MODEL

3.5.1 Code Description

The FE3DGW code (Gupta et al., 1979, PNL-2939) simulates three-dimensional, time-dependent water flow in fully saturated porous media. The code can represent single-layered systems of variable thickness or multilayered systems in which the number of layers (up to 20) and the thickness of each layer can be varied. Hydrologic conductivity can be anisotropic and inhomogeneous. The groundwater and the porous media it saturates are both taken to be compressible. It is assumed that the porous matrix material does not dissolve in water.

Input consists of the geometry of the finite-element network at surface level; well log data at each node; descriptions of layer depths and thicknesses, and geologic properties within each layer (hydraulic conductivity tensor, porosity, and compressibilities); boundary conditions; and time steps. Output consists of flows and the hydraulic head as functions of time and of position in the region being simulated. The output is obtained by solving an equation proposed by Jacob (1950) for three-dimensional transient flow. This equation is solved by a finite-element approach, which can accommodate the irregular boundaries that often occur in geologic systems. The FE3DGW code is limited

to simulating saturated media. It is written in FORTRAN IV-Plus and is operational on a PDP 11/45 computer.

3.5.2 Development Stage

FE3DGW is ready for use on a PDP 11/45 computer.

3.5.3 Documentation

The FE3DGW code is documented in PNL-2939, which includes a user's manual and a program listing. While the documentation is generally good, it is not quite in the NUREG-0856 format (Silling, 1983), as indicated by the following points.

1. It does not include a standard software summary.
2. It does not have a separate section in which the assumptions and limitations of the code/model are summarized and discussed.
3. Boundary conditions appropriate to Jacob's (1950) equation are inadequately described, as are the means for introducing those conditions into the Galerkin finite-element formulation used by the code.
4. There is no separate section on code validation.
5. With respect to code assessment and support, there is no separate section on past and possible future model reviews, nor is there a chronology of code versions.

The following typographical error in PNL-2939 should be corrected, namely, H_0 and U_0 should be interchanged in the definitions on page 63. Also, the term "drawdown" should be defined.

3.5.4 Performance Specification Review

Performance specification review has not been completed.

3.5.5 Code Design Review

The only code design review is the one conducted by the code developers.

3.5.6 Verification

The FE3DGW code has been verified by comparing its solutions to analytic solutions in three cases: (1) time-dependent radial flow to a well pumping at a constant rate in an infinite, homogeneous, and isotropic aquifer; (2) steady state, two-dimensional flow through a rectangular aquifer with a reservoir having a head 25 feet above the water table; and (3) time-dependent, radial flow to a well pumping at a constant rate from an elastic aquifer confined by semipervious elastic strata.

Agreement between the FE3DGW-generated solutions and the analytic solutions was close in the first two cases and generally close in the third. In the first case, the values of drawdown as a function of time obtained from the code are consistently slightly less than those obtained from the analytic solutions. This difference, while small, should be explained. In the second case, agreement was excellent. In the third, agreement was very close, except at early times in the subcase of a radius of 7.389 meters. There, the discrepancy was about 10% and should be explained. Was it due to the finite time intervals. Would the discrepancy be even greater at larger radii?

These three cases pertained to geologic systems in which, because of symmetry, the solution to Jacob's (1950) equation depends on less than three spatial variables: one variable in the first case, two in the second, and one in the third. Thus, the full, three-dimensional, time-dependent capability of the code has not been verified. Indeed, for the first and third cases, which involve time dependence, there was only one spatial variable, radial distance. Hence, the FE3DGW code needs further verification. In particular, its full three-dimensional, time-dependent capability should be verified. To do this will probably require a benchmarking test against another code.

3.5.7 Validation

No validation tests were reported in PNL-2939.

3.5.8 Proposed ONWI Application

Because the FE3DGW code will be used by ONWI to simulate the flow of groundwater to and away from the waste repository, it is a site assessment code.

3.5.9 Relationship of Model to Other Codes

The FE3DGW code does not require input data from other codes. However, it does require the use of supporting programs to verify input data. These supporting programs are part of the FE3DGW package. The output flows could, with appropriate adaptation, be used as input to radionuclide transport codes like MMT and LAYFLO.

3.5.10 Application of Code to Other Problems

The FE3DGW code has been used to simulate water flow through aquifers in the Sutter Basin in California (Gupta and Tanji, 1976) and flows under Long Island in New York (Gupta and Pinder, 1977).

3.5.11 Suitability of Model for Salt Repository Application

The FE3DGW code is suitable for simulating the flow of water to and away from a salt formation. It is probably not suitable for simulating flow through a salt formation, because the model does not take into account the absorption of water by the salt or the dissolution of salt by the water.

3.5.12 Peer Review

The FE3DGW code has not been subjected to peer review.

3.5.13 References for Section 3.5

Gupta, S.K., and G.F. Pinder, *A Three-Dimensional Finite-Element Model for Multi-layered Groundwater Reservoir of Long Island, New York*, Department of Civil Engineering, Princeton Univ., Princeton, N.J. (1977).

Gupta, S.K., and K.K. Tanji, *A Three-Dimensional Model Galerkin Finite-Element Solution of Flow through Multi-Aquifers in Sutter Basin, California*, Water Resources Research, 12(12):155-162 (1976).

Gupta, S.K., et al., *Finite-Element Three-Dimensional Ground-Water (FE3DGW) Flow Model Formulation, Program Listing and User's Manual*, Battelle Pacific Northwest Laboratories, Richland, Wash., PNL-2939 (1979).

Jacob, C.E., *Engineering Hydraulics*, H. Rouse, ed., Chapter 5, John Wiley and Sons, New York, N.Y. (1950).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

3.6 FFSM: FAR FIELD STATE MODEL

3.6.1 Code Description

The FFSM code (INTERA, 1983, ONWI-436) predicts the approximate geologic and climatic state of a nuclear waste repository site over thousands of years. Such a

model is necessary for repository performance assessment in view of U.S. Environmental Protection Agency and NRC requirements that DOE provide "reasonable assurance" that escaped radioactivity will be within specified limits (thousands of meters from the waste packages) at the perimeter of a repository site within a 10,000-year period. Meaningful site simulations may involve areas as large as 10,000 square kilometers (p. 187)* and periods as long as 10 million years (p. 12). Such spatial/temporal considerations necessitate development of a model based on probability theory. Such a model will be considerably different in form from those employed for simulations of waste package and repository processes in that it will not be verifiable in the usual sense of the word.

The FFSM code attempts to represent quantitatively a number of geologic and climatic conditions throughout a waste isolation site and to treat natural and man-induced changes in these conditions within a probabilistic framework. It accounts for cumulative and interactive effects of multiple phenomena. Submodels of FFSM predict the occurrence of, or simulate the effects of, undetected features, climatic changes, resumption of worldwide glaciation, local glaciation, folding, salt diapirism, magmatic events, faulting, regional deformation, geomorphic processes, dissolution fronts, breccia pipes, solution mining, and future drilling activities. The relationships of FFSM to the biosphere and geosphere realms and the relationships of these realms to the repository and waste package environments are shown in Figs. 5 and 6. The term

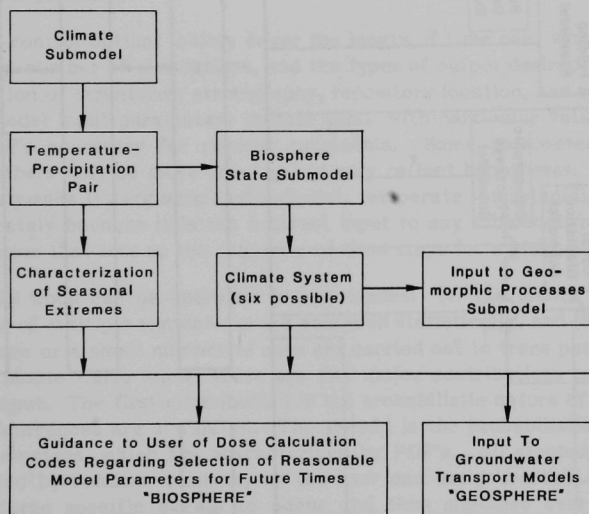


FIGURE 5 Relationships between Climate and "Biosphere State" Submodels and Their Uses for Simulations in the Biosphere and Geosphere Realms

*Page numbers in Sec. 3.6 are from ONWI-436.

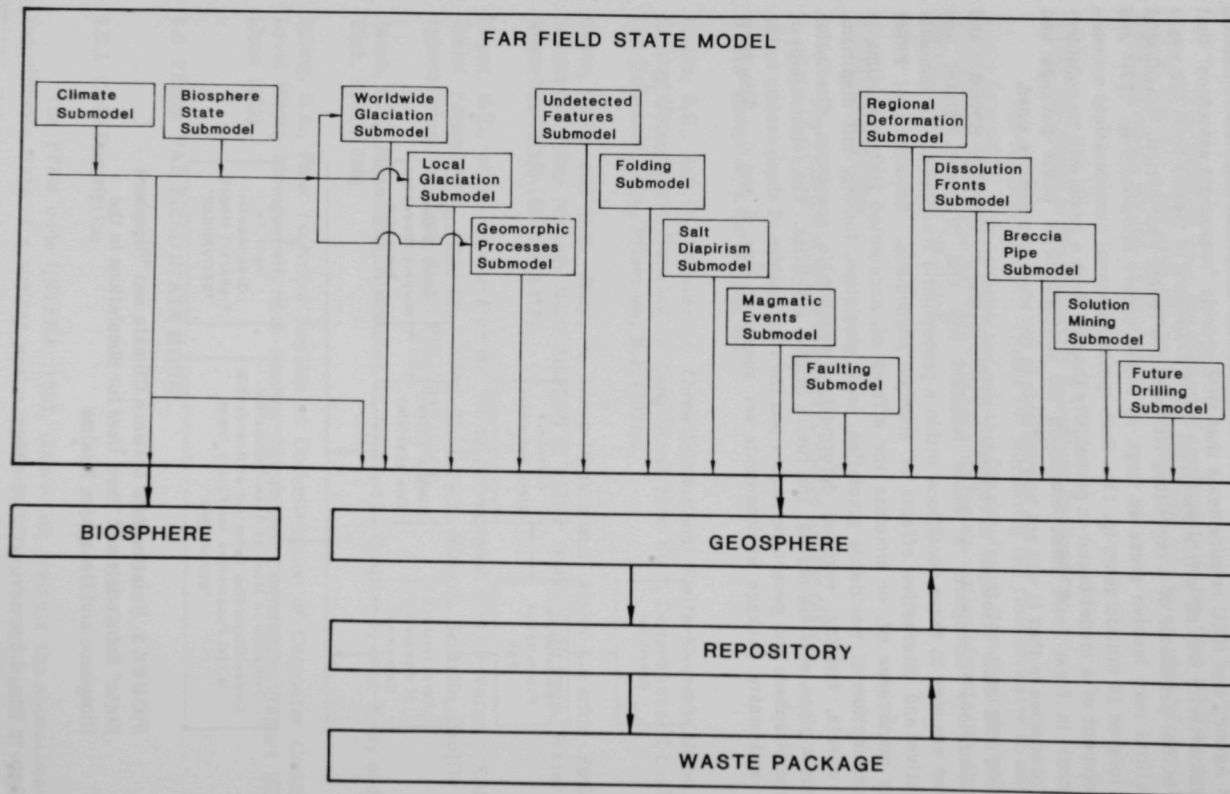


FIGURE 6 Relationship of the FFSM Code to the Biosphere and Geosphere Realms Being Addressed and to the Repository and Waste Package Environments

"biosphere state" is something of a misnomer because the submodel does not describe or simulate a biosphere state; it merely classifies the local climate at a site.

Simulation of a repository site requires use of input parameters that are either variable or uncertain. The FFSM code handles this problem by defining probability density functions (PDF's) for the parameters. Other inputs are inherently probabilistic, such as the probability of occurrence of a certain kind of event. Thus, the output parameters of FFSM simulations will be random variables with their own PDF's. However, these variables are too complicated to be calculated because of the large number of probabilistic input parameters. Instead of mathematical or analytic calculations, the FFSM code uses a Monte Carlo simulation approach to model long-term changes in the site or the probability of occurrence of specific conditions. In such an approach, selection of random numbers with certain statistical properties is used as an analog to selection of specific parameters. Then, by repeated simulations, one infers the overall behavior of the system. "For example, if on 1000 independent simulations of system evolution, the elevation of a given reference point never varies by more than 10 meters, then one can estimate that the probability is less than one in a thousand that the reference point elevation will vary by more than 10 meters during site evolution" (p. 20).

The following kinds of information are required as input to the FFSM code: (1) program control options, (2) site geometry, (3) submodel input parameters, and (4) worldwide climatic state sequence.

Program control options mainly cover the length of time over which simulation is to take place, the number of simulations, and the types of output desired. Site geometry covers specification of structures, stratigraphy, repository location, and reference points on rivers. Submodel input parameters include some with particular values and some in the form of PDF's necessary for running submodels. Some parameters may be site specific, while others may be more universal or may reflect hypotheses. The worldwide climatic state sequence (interglacial, interstadial, temperate interstadial, and stadial) is considered separately because it is not a direct input to any submodel, but is input to a time step subroutine that sets up the sequence of time steps for a given simulation.

The FFSM code can be operated in two modes: (1) the Monte Carlo mode, in which the results of multiple simulations are analyzed statistically, and (2) the single-run mode, in which one or a small number of runs are carried out to trace particular kinds of effects. In the Monte Carlo mode, there are two major contributions to the stochastic nature of the output. The first contribution is the probabilistic nature of certain events, whose actual occurrences are simulated. The second is the probabilistic description of many model parameters, which are characterized by PDF's. All stochastic aspects can be fully simulated by random numbers, or the user can assign certain values to some parameters or force specific events to occur and then simulate over the remaining values.

To give examples of input and output parameters is beyond the scope of this summary. However, the sample problems presented on pages 187-221 illustrate how FFSM operates for:

1. Four submodels not requiring intercommunication.

2. Six submodels, some of which are interdependent.
3. All of the submodels.

A feeling for the nature of an FFSM simulation can be gained from sample problem 1 above. The simulation results (probabilities) given correspond to the following questions.

<u>Question</u>	<u>Probability</u>
What is the probability of at least two undetected boreholes?	0.60
What is the probability of at least one volcanic vent by the year 15,000?	0.20
For what fraction of years is the precipitation rate greater than 1200 millimeters?	0.02
What is the probability that the annual precipitation rate is between 1000 and 1200 millimeters per year?	0.40

Application of the FFSM code to a salt repository site will be an iterative process. Validation of initial results will be by peer review (p. 3), a process by which knowledgeable experts on each submodel will pass judgment on the reasonableness of the results. The authors of ONWI-436 discuss the following additional limitations of the FFSM code.

1. Large quantities of data are necessary to carry out a simulation for a specific site.
2. Many simulations are necessary to gain useful information concerning all but the most likely occurrences or perturbations at a particular site.
3. The model does not contain a groundwater component that permits the results of simulations to be summarized in terms of the effects on the groundwater regime.
4. The code will need to be modified and upgraded for application to specific salt sites.

The FFSM code is written in ANSI FORTRAN 77. It has been run on a CDC tandem system of a CYBER 720 (NOS) and a CYBER 7600 (SCOPE). Core storage requirements on the CDC system for the program are 111,000 octal words (small core memory) and 450,000 octal words (large core memory).

3.6.2 Development Stage

The FFSM code is based in part on Battelle Pacific Northwest Laboratories' Geologic Simulation Model (GSM) (Petrie et al., 1981; Stottlemire et al., 1981). The model and code, which are entirely new, were developed for INTERA by Arthur D. Little, Inc., and are structured for general application rather than for simulations at salt sites. As stated on page eight: "Since the model considers a broad set of natural and human phenomena, for a detailed specific site simulation, the code may need to be modified and upgraded." While this statement is correct, it doesn't go far enough in that certain of the submodels also need varying amounts of developmental work before the model can be said to be ready (see Sec. 3.6.4).

3.6.3 Documentation

The following exceptions to, or gaps in correspondence with, NUREG-0856 (Silling, 1983) documentation guidelines are noted.

1. The applicability of the model to salt sites is not specifically discussed.
2. The overall performance of the entire model, although discussed with reference to two test problems, is not presented in a convincing fashion.
3. The limitations of the component models are not discussed.
4. General rules or recommendations for use of the submodels are not given.
5. Sample problems that have been run do not exercise a large part of the code.
6. Plans for independent review of the model or submodels are not given.
7. Plans for updating software summaries, documenting revisions, reporting of errors, describing updates and new versions, and responding to NRC questions need to be spelled out.

3.6.4 Performance Specification Review

As mentioned above, ONWI-436 does not adequately describe the analysis to be conducted for bedded or domed salt repository sites. Although a performance specification review was conducted for GSM, FFSM's predecessor, for results of the GSM's application to the Pasco Basin in a basalt terrain, no performance specification review has been conducted for a salt site. The GSM review illustrated the feasibility of obtaining

the data required for far-field-type simulations and "suggests the usefulness of this approach for making long-term probabilistic predictions of the evolution of a potential repository site" (p. 83). When a performance specification review is conducted for application of the FFSM code to a salt site, the issues given below should be considered. (Some of these issues are also discussed in Sec. 12.3 of Harrison et al. (1984). That preliminary discussion has been revised and augmented here.)

Climate and Biosphere State Submodels

The Climate Submodel attempts to describe local climatic parameters as these are affected by worldwide climatic states. The time sequence of worldwide climatic states must be supplied by the user. "This sequence is first acted upon by the Time Step Margin Subroutine of the main system program, with the result that a single climate state is associated with any simulation time step. For each time step, values of mean annual precipitation and temperature are chosen from combinations found throughout the world today; an inconsistent pair is discarded and a new one picked" (p. 25).

A change in one of four possible global climate states treated in the model is expressed at a particular location by changes in precipitation and temperature. Values for mean-annual precipitation and temperature are selected for each time step off of PDF's of predicted mean-annual precipitation and of predicted mean-annual temperature input by the user for each of four climate states. Historical correlations between local climate and worldwide climate using information on pollen and lake-sediment analysis form the basis for each PDF. If a temperature-precipitation pair is not consistent with the ranges found throughout the world at present, another pair is selected using the PDF's. In addition, an index for seasonal extremes for each climate pair is entered by the user, as defined on page 27.

The Biosphere State Submodel classifies the climate system at the site based on precipitation and temperature values chosen in the Climate Submodel. One of six climate systems, based on a classification by Wilson (p. 52), is selected at a given time step. The Wilson classification is correlated with the Köppen climate classification. Relationships between the Climate and Biosphere State submodels, and their uses for simulations in the biosphere and geosphere realms, are shown in Fig. 5.

The following aspects of the above-described Climate and Biosphere State submodels should be considered in any performance specification review for application of the FFSM code to a salt site. It is inappropriate to use only mean annual data to specify a climate in the Climate Submodel. Variance of both temperature and precipitation during the seasons is of utmost importance for specifying botanic and geomorphic responses. Further, the Wilson and Köppen climatic classification systems are poor choices for the Biosphere State Submodel. The Köppen classification was derived about 80 years ago. Although still widely used in introductory textbooks, it is coarse, antiquated, and empirically based. A better method for arriving at local climates would be one based on physical principles.

An apparent oversight in the description of the Climate Submodel is a reference to how future climatic parameters will be determined. The statement in the first

paragraph of page 25 that the forecast values of the climatic parameters are to be checked for consistency against values found throughout the world today arbitrarily assumes that future climates will be composed solely of those in existence today. It must be remembered that some of the climatic characteristics from as little as 13,000 years ago have no analog in today's climate.

Predictions of future climates should be derived from models that calculate climate as a function of changes in long-term solar/earth radiation and energy balances. The Milankovitch periodicities of the earth's orbital characteristics around the sun should be taken into account. These periodicities range from about 10,000 years to 90,000 years and have been shown by the CLIMAP research to explain most of the variance in paleo-climates over the last several hundred thousand years. Therefore, they could be used as a predictor for the next like interval of time, although they would have to be modified to take into account changes in land use, warming resulting from increased carbon dioxide in the atmosphere, changes in surface albedo, and other relevant factors.

If future changes in radiation are predicted based on the Milankovitch equations, temperature equilibria at the earth's surface can be estimated, yielding values that could be outside the range of those presently measured. Although latitudinal advection also influences temperature, for a first approximation, the effect of future advection may be assumed to be equivalent to that of today. Evidence strongly suggests that the centers of large-scale surface circulation systems were essentially constant throughout the Holocene and Pleistocene (Bryson and Wendland, 1967; Wendland and Bryson, 1978). In other words, subtropical anticyclones over the oceans, winter subpolar anticyclones over high-latitude continents, and subpolar cyclones over high-latitude oceans will undoubtedly remain at about their present locations well into the future. One may therefore assume that the circulation pattern about these centers will also remain essentially unchanged (Bryson, 1966; Wendland and Bryson, 1980).

The advantages of using a physical model for predicting climate are obvious. A much more credible product will result than would result from predicting mean temperature and precipitation data from a statistical model.

Developing a model to predict the radiation budget as a function of the Milankovitch periodicities is relatively easy, because the algorithms have already been developed and explained (Berger, 1978). Translating the radiation budget into specific climatic parameters is more difficult but can be done. Even if the methodology to predict the climatic parameters from Milankovitch periodicities is regressive, it is at least as credible as what is proposed in ONWI-436 and has the advantage of being physically based. The importance of a physical model cannot be emphasized too strongly, because the climatic research community will appropriately reject long-term predictions based only on present analogs and, in particular, those based on empirical systems like Wilson's or Köppen's.

The discussion at the top of page 27 assumes a constant correlation between local and global glaciation. Climate forecasts for tens or hundreds of thousands of years into the future cannot be so restricted.

When discussing the Biosphere State Submodel on page 51, mean temperature and precipitation are again mentioned as the only climatic predictors (also see Fig. 2-14). The radiation gradient must be added, as must humidity, since these parameters are important in estimating the work done by weather/climate on a geomorphic surface.

Geomorphic Processes Submodel

The Geomorphic Processes Submodel simulates the reduction in elevation of the surface of a repository site as a function of gradual or catastrophic erosion. On page 60, ONWI-436 states:

Gradual erosion affects land and river points. Rates of gradual erosion are a function of climate system, values of and seasonal extremes in precipitation and temperature, and surface deformation by faulting, folding, or regional deformation. Catastrophic erosion primarily affects rivers that carry glacial flood water during glacial melting, and rivers that discharge into the sea during changes in sea level.

Both types of erosion are specified initially in the model input for average erodibility and are then scaled relative to the erodibility of the uppermost rock unit. Both the thickness of the uppermost unit and the surface elevations of all points are then decreased by the scaled value for erosion. Different rates of erosion apply for each of the six climatic systems.

Catastrophic erosion pertains to processes associated with changes into or out of climate state 4. This climate state is described on page 26 as follows: "STADIAL CLIMATE -- a substage of a glacial stage marked by glacial advance, maximum extent of continental glaciation, areal extent of glaciers 25-35%." The idea here is that as the climate cools and glaciers grow, sea level lowers and downcutting streams reduce the elevation of the site surface. Then, "as the climate warms, glaciers melt causing large volumes of sediment-free water to flow away from the glacier terminus. This melt-water [sic] will erode the beds of rivers through which it flows. These factors are included in the submodel" (p. 61).

The rate of lowering of the land surface is estimated by entering into the model predicted denudation rates, for each of the six Wilson climatic systems, in the form of a PDF for removal of a rock of average erodibility (e.g., sandstone). The submodel then operates on this PDF, developing a scaled erosion rate that "is then subtracted from the elevation, relative elevation, and thickness of the top layer for each point" (p. 61).

The submodel also accounts for accelerated erosion caused by river downcutting while the site area is being uplifted. "Since uplift caused by deformation is itself a gradual process, over large periods of time, rates of river downcutting can be expected to keep up with rates of uplift. The amount of erosion is thus assumed to equal the sum of all uplift processes" (p. 61).

For catastrophic erosion, PDF's must be entered for the erosion of river beds anticipated during either climatic change. Values for either PDF are estimated from

average erosion during previous climate changes. The selected erosion rate for either type of catastrophic erosion is then modified according to the erodibility of the uppermost layer at each river point, and the resultant erosion rate is then subtracted from the thickness of the uppermost layer and the relative elevation of each river point.

The Geomorphic Processes Submodel would benefit from a review by a panel of geomorphologists. For example, gradual erosion is probably intended by the author of the submodel to be equivalent to geologic erosion, but this equivalency is unclear. Use of the term "catastrophic erosion" to describe erosion by "glacial meltwaters" or by "coastal drainages under conditions of lowered base level" is exaggerated. These kinds of fluvial erosion would in no way approach magnitudes suggested by the term "catastrophic." For example, formation of channeled scablands by rapid drainage of glacial Lake Missoula would be considered to be a catastrophic event. Catastrophic events are one-of-a-kind events of extreme rarity. Furthermore, glacial meltwater is not free of sediment, as stated by the authors, but contains high concentrations of suspended sediment. Although some channel incision could logically be assumed to result from the influx of large volumes of meltwater, most such events are accompanied by accumulations of large quantities sand and gravel, which indicates a depositional rather than an erosional mode.

The Geomorphic Processes Submodel interfaces with submodels pertaining to uplift, including folding, faulting, and regional deformation. The model assumes that uplift will result in increased erosion and stream incision. However, depending on the spatial relationship between existing drainage systems and the area of uplift, an increase may not occur. For example, if uplift occurs in the downstream portion of a larger drainage basin, erosion will be reduced. In particular, if one were looking at the effects of renewed activity along the Nemaha Uplift on the Platte River system, uplift would not result in increased denudation.

ONWI-436 also assumes that the amount of erosion is equal to the sum of all uplift processes and that rates of downcutting keep up with rates of uplift over long periods of time. Although such assumptions may be required to simplify the model, they cannot be substantiated in the geomorphic literature. The elements of time and geomorphic response enter into the problem. Schumm (1963) reported average denudation rates of 0.1-0.3 feet per thousand years, with a maximum of 3 feet per thousand years, and an average modern rate of orogeny of about 25 feet per thousand years. Other geologic evidence indicates that the rates of uplift and downcutting are sometimes different.

The effects of climatic change are also much more complicated than the treatment afforded by the model. The effects of climatic conditions on erosion and sediment yield are discussed by Langbein and Schumm (1958) and Schumm (1965, 1968), among others.

Finally, the amounts and types of input required by the user seem unrealistic. Data may not be available to generate a PDF for the erodibility of various rock types. (A point of confusion, however, is that the input for this category as shown on page 173 is a simplified scale of "relative" erodibility.) Consequently, poor input will certainly result in poor output. If the user knew denudation rates for all of the climatic types and for all of the rock types in the area, he would have little need for the Geomorphic Processes Submodel and could make direct computations of erosion.

Folding Submodel

The Folding Submodel simulates the growth of synclinal or anticlinal folds within the site area. The user provides the location of real or hypothetical folds, and the model changes the elevation of points on them, according to a selection from a PDF. This simulation process can take place over three distinct time intervals, using different input data to reflect that regional tectonic changes may imply different folding conditions over the simulation period. Fold growth can also affect the rate of faulting in the Faulting Submodel.

Within the time framework of the model, folding such that surface features might be affected would appear to be unlikely in all but tectonically active areas. For the 10,000-year period germane to NRC licensing requirements, the probability that this type of folding could affect the salt sites under active consideration appears exceedingly low. Therefore, it will be extremely conservative, in a geologic sense, to apply this submodel to particular salt sites.

The discussion of the Folding Submodel does not address the possibility of using this submodel to simulate formation or reactivation of salt domes; processes that could affect surface features. Such surface disturbances could be the end result of diapirism as discussed in Sec. 2.7.6 of ONWI-436. It would seem possible to simulate a dome rising at depth by choosing fold axis coordinates that are relatively close together. The geometry of the resulting fold would be that of an elongate dome. For salt dome sites under consideration, the application of this submodel to salt dome formation appears to be more relevant over the next 10,000 years than the application of the submodel to tectonically induced folding. The example of subsidence caused by removal of subsurface fluids is not appropriate for the Paradox or Palo Duro basins but may be relevant for some of the candidate salt domes.

Local Glaciation Submodel

The Local Glaciation Submodel simulates the movement of a continental glacier assumed to be covering part of the study area. It models the glacier's effects on point elevations as a result of isostatic response and on the occurrence of faulting. Because the bedded and domed salt sites presently under consideration for repository development were not subject to continental glaciation in the past, this submodel is irrelevant unless modified to include the effects of mountain glaciation. Even for the Paradox Basin sites in Utah, however, a threat from renewed mountain glaciation is probably of little consequence. For example, the lowest known altitudes of cirque floors in the La Sal Mountains southeast of Moab is 2900 meters, and the lowest known altitude reached by glaciers on the Aquarius Plateau to the west is 2000 meters. It is doubtful that the Local Glaciation Submodel has any relevance to the salt sites under consideration, either in terms of the direct action of glacial loading or ice erosion.

Magmatic Events Submodel

On page 42, ONWI-436 states:

The Magmatic Events Submodel simulates the occurrence of one or more volcanic vents within the study area, on the basis of a user-supplied probability. The location of such vents is simulated based on pdf's for x and y coordinates. For vents within certain specified distances of the repository point, releases are identified either to the air and land surface (through the vent itself) or to other subsurface strata (due to associated intrusive movement).

It appears that the authors of ONWI-436 confused or combined two types of igneous events -- magmatic and volcanic. Volcanic events might be more relevant for sites on the Columbia Plateau, whereas the rise of magma as an intrusion might be more applicable for salt sites. A good example is the inferred magma rise (intrusion) below the Long Valley caldera in Mammoth Lakes, Calif., which has resulted in an area of uplift and seismic activity (Kerr, 1983). As far as potential salt sites are concerned, areas where magmatic events that have the potential to disrupt a repository could occur have essentially been screened out. The assumption that a magmatic event is characterized first by the occurrence of a volcanic event (p. 42) appears faulty for the reasons stated above. Also, ONWI-436 must explain how volcanic activity would be relevant to the Biosphere State Submodel.

3.6.5 Code Design Review

Code design review appears to have been conducted by the authors of ONWI-436, but details are lacking.

3.6.6 Verification

Three test problems were run as an exercise in code verification. Perfect agreement was found between the results of the test problems and those expected on the basis of hand calculations. Sample problem 1 used four submodels that did not involve interdependence. Sample problem 2 used 10 submodels, many of which were interdependent. Sample problem 3 exercised all submodels. The results of this last problem showed that all data were read in correctly and that all submodels operated properly. No plans are presented in ONWI-436 for further verification activities.

3.6.7 Validation

The FFSM model has not been validated, and it will be impossible to validate in the classic sense. At present there are no specific plans for validation. It is suggested in ONWI-436, however, that the validation approach used in Foley et al. (1983) for the Geologic Simulation Model, the FFSM code's precursor, could be applied to validation of

the FFSM code. In other words, validation would be accomplished by peer review of model input and of the results of modeling runs.

3.6.8 Proposed ONWI Application

The FFSM code is to be used for site assessment. It is expected to cover the next 10,000-1,000,000 years and be useful for predicting climatic and geologic phenomena over horizontal distances of tens of kilometers. Input parameters (e.g., event probabilities, site characterization parameters, and estimates of future human intrusions) are given in terms of PDF's or as single values, depending on data availability and associated uncertainties (see Sec. 3.6.5).

3.6.9 Relationship of Model to Other Codes

The FFSM code is based on a stand-alone model.

3.6.10 Application of Code to Other Problems

The precursor to FFSM, the Geologic Simulation Model, was applied to a reference site in Columbia Plateau basalt (Foley et al., 1982).

3.6.11 Suitability of Model for Salt Repository Application

The FFSM code is not presently suitable for the salt repository application (see Sec. 3.6.4).

3.6.12 Peer Review

The FFSM code has not undergone peer review for either verification, validation, or application activities.

3.6.13 References for Section 3.6

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3.7 FTRANS: A TWO-DIMENSIONAL CODE FOR SIMULATING FLUID FLOW AND TRANSPORT OF RADIOACTIVE NUCLIDES IN FRACTURED ROCK

3.7.1 Code Description

The FTRANS code (INTERA, 1983, ONWI-426) simulates fluid flow and dissolved radionuclide transport in fractured and unfractured (granular) porous media in two dimensions. The code consists of two separate components: a fluid flow code and a solute transport code. The fluid flow model assumes incompressible flow and steady state boundary conditions, and applies to a single, confined aquifer, that is, one bounded by overlying and underlying impermeable formations. The differential equation governing fluid flow assumes Darcy's Law is applicable and is solved using a two-dimensional Galerkin finite-element method. The solution provides the Darcy velocity components required as input to the solute transport model equations.

The differential equations governing solute transport account for Darcy flow, linear isotherm adsorption, radioactive decay chains, and transport through fractured and unfractured porous media. They are solved using a combination of a two-dimensional, upstream-weighted-residual, finite-element technique and a one-dimensional Galerkin finite-element method.

Fractured porous media of low permeability are treated using a dual-porosity approach; that is, they are assumed to contain many fractures. Such media are idealized as a fracture continuum in which a matrix of rectangular or spherical matrix blocks is embedded. Transport through the fracture continuum is assumed to be by both advective and dispersive mechanisms, while transport within the matrix blocks is by Fickian diffusion. Transport back and forth between the matrix blocks and the surrounding fracture continuum is also accounted for.

Fractured porous media of high permeability are treated by a discrete fracture model that assumes only a few discrete fractures in a continuum rock matrix. Diffusive transport is accounted for in the rock continuum, and both advection and dispersion are considered within each individual fracture. This approach requires input data on the geometry of each individual fracture plane.

Problems that can be addressed with the code include transport of radionuclides in both near- and far-field porous media surrounding a waste repository. Flows into wells that fully penetrate aquifer systems also may be analyzed. Limitations include no treatment of thermal or mechanical deformation effects on the flow field. The boundary conditions for the flow model must include overlying and underlying impermeable formations and steady state conditions. Two-phase flows are not permitted, and chemically reactive solute systems cannot be treated.

The code was written in FORTRAN IV for a CDC machine and could presumably be readily adapted for use on other hardware. The code has approximately 2000 source statements.

3.7.2 Development Stage

A newly developed code, FTRANS is operational on a CDC-CYBER 176 system. It was originally developed for use on CDC machines by Huyakorn at Geotrans, Inc., and revisions and modifications were made by INTERA (1983) for ONWI. The changes made by INTERA include correction of minor coding errors and integration with other INTERA codes. The code has not been used extensively or reviewed by personnel outside the ONWI program.

3.7.3 Documentation

The code is well documented in ONWI-426 and is in accordance with the requirements of NUREG-0856 (Silling, 1983).

3.7.4 Performance Specification Review

The performance specification review was conducted by INTERA and is documented in ONWI-426. No major problems or deficiencies were noted. Model limitations include no treatment of thermal or mechanical deformation effects, essentially incompressible flow, Fickian diffusion, and linear isotherm adsorption. ONWI-426 states that the requirement for specific fracture geometry for the discrete-fracture approach may limit its application.

3.7.5 Code Design Review

Code design review is covered by INTERA in its documentation of FTRANS in ONWI-426.

3.7.6 Verification

ONWI-426 describes six example problems to which the code was applied. Because four of these involved comparison with published analytical solutions, they constitute code verification tests. Of these four, two were concerned with transport within aquifers and two with radial flow within an aquifer to a fully penetrating well. The results are summarized as follows:

1. One-dimensional transport of a three-membered radioactivity chain in a homogeneous, porous medium. This problem tests the upstream weighting and Galerkin numerical scheme coding, the chain reaction equation coding, and the time-dependent flux boundary conditions of the solute transport model. Agreement with published analytical solutions was excellent.
2. Two-dimensional transport of a parent radionuclide species in fractures, with diffusion into rectangular matrix blocks. This

problem tests the finite-element formulation and numerical scheme for handling transport in a fractured medium by using the discrete-fracture representation. For concentration distributions along the fracture, agreement was excellent. Agreement for distributions on a cross section of the matrix block was not as good. In general, agreement improved with increased simulation time. For this particular problem, the dual-porosity approach was slightly more accurate than the discrete-fracture one because it ignored longitudinal diffusion as did the analytical solution.

3. Radial flow to a fully penetrating well into a parallel fractured (horizontally) aquifer system with transverse leakage from adjacent matrix to fracture. Comparison of drawdown versus time showed good agreement with the analytical solution for long times, but poorer agreement for shorter times. A finer mesh size improved the agreement over shorter times.
4. Radial flow to a well in a confined aquifer containing a single vertical fracture. Results were similar to those in problem 3.

None of the verification tests involved the ability of the code to handle multilayered aquifer systems..

3.7.7 Validation

Because FTRANS is a newly developed code, there has been no validation to date.

3.7.8 Proposed ONWI Application

ONWI proposes to use FTRANS for analysis of fluid flow and radionuclide transport through porous and fractured media in the vicinity of the waste package. Other applications are not mentioned. In view of the nature of a salt repository, it is likely that FTRANS would be applicable only for special assessments involving flows outside of the salt deposit or in the salt deposit but only after it has been saturated.

3.7.9 Relationship of Model to Other Codes

FTRANS can be operated as a stand-alone code. However, it does require a number of inputs that could be provided by other codes. In particular, it requires information on flow fields in cases where deformation has an influence on fluid capacity or on the flow field. In such cases, STAFAN, which treats coupled flow/deformation processes, could provide the input velocity field to FTRANS. In addition, FTRANS requires information on solution speciation that could be provided by source codes like WAPPA combined with geochemical codes like EQ3/EQ6 or PHREEQE.

3.7.10 Application of Code to Other Problems

Other than the six example problems referred to in Sec. 3.7.6, no other applications of FTRANS are known.

3.7.11 Suitability of Model for Salt Repository Application

The suitability of the FTRANS code for the salt repository application has not been addressed in any of the ONWI documents. Given the relatively impermeable and plastic nature of salt, it is not obvious what role FTRANS will play in near-field repository assessment. Because it cannot account for thermal effects, its utility is limited for the near field. It could conceivably be used to analyze fluid flows and radionuclide transport after the repository is saturated as long as proper care were taken to incorporate thermal and deformation effects and if the proper boundary conditions could be specified. FTRANS could also be used in far-field applications (e.g., outside of the salt deposit) to analyze either the movement of water to the salt deposit or the transport of radionuclide solutes away from an already saturated salt deposit and breached waste package.

3.7.12 Peer Review

No external peer review has been documented. Emphasis in such a review should be on the code's applicability to salt repository performance assessment.

3.7.13 References for Section 3.7

INTERA Environmental Consultants, Inc., *FTRANS: A Two-dimensional Code for Simulating Fluid Flow and Transport of Radioactive Nuclides in Fractured Rock for Repository Performance Assessment*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-426 (April 1983).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

3.8 GEOTHER: A TWO-PHASE FLUID FLOW AND HEAT TRANSPORT CODE

3.8.1 Code Description

GEOTHER (INTERA, 1983, ONWI-434) simulates one- or two-phase flow of pure water and heat transport in up to three dimensions in porous media. Either Cartesian or cylindrical coordinates may be selected. It was designed for use in geothermal reservoirs, but it could be used to evaluate the effect of heat generated by the waste form in the vicinity of the waste package. The model assumes thermodynamic

equilibrium between the porous rock medium and the fluid (liquid and vapor phases of pure water). Cubic spline functions are used to represent the empirical relationships between the thermodynamic properties of the fluid. Pressure and enthalpy must be determined by solving two nonlinear partial differential equations. These governing equations are reduced to finite-difference forms that are solved iteratively by a Newton-Raphson method for each time step. The iterative solution scheme involves the solution of a nonsymmetric matrix. The code employs a slice-successive overrelaxation procedure to solve this matrix.

ONWI-434 lists 12 assumptions or limitations inherent in the model. Of these, the following five should be of special concern to users:

1. Capillary pressure effects are ignored.
2. Thermal equilibrium is assumed to exist between steam, liquid water, and rock.
3. Only pure water is considered.
4. Darcy's equation for multiphase flow is assumed.
5. Kinetic and potential energy are ignored, as is the pressure material derivative (compressible work term).

Additional important limitations noted in ONWI-434 include:

1. Only pure water is assumed in the thermodynamic relationships.
2. A statement that well-bore calculations cannot be performed contradicts the use of well-bore-type test problems as described in the text.
3. Unless fractures are treatable as part of the porous media, the model is not applicable. Single fractures with simple geometry can be treated as indicated in a test problem.
4. The model has no thermomechanical capabilities. However, the code output could be used as input to a mechanical code to compute stresses.
5. The temperature range is limited by the applicability of the empirical thermodynamic relationships to 10-300°C.
6. The model is not able to handle concentrated solutions of any chemical or radiological species. Hence, its applicability to waste packages stored in salt repositories is quite limited.

The code was written in FORTRAN IV for use on a CDC CYBER 176 machine. It consists of about 3000 source statements.

3.8.2 Development Stage

GEOETHER is a fully operational and documented code. Earlier versions have been described by Faust and Mercer (1979a, b).

3.8.3 Documentation

The GEOETHER code documentation is generally in accordance with NUREG-0856 (Silling, 1983), with the exception of the items discussed below. The theory section is very brief and contains only the final governing equations. Although reference is made to more detailed discussions and derivations, this section should be expanded to make it somewhat more self-contained. Also, the section on model verification is inadequate. Of the six test problems listed, only two have analytical solutions. The results of comparing GEOETHER results with the analytical results for these two problems are not reported. Results for two other test problems used for intercode comparison studies are presented in some detail, but the test results do not constitute satisfactory verification of the GEOETHER code (see Sec. 3.8.6).

3.8.4 Performance Specification Review

The performance specifications are briefly reviewed in the theory section of the GEOETHER code documentation prepared for ONWI-434. No additional external review is documented.

3.8.5 Code Design Review

The review of the code design by INTERA is incorporated into their documentation of the code in ONWI-434.

3.8.6 Verification

ONWI-434 cites Stanford Geothermal Program (1980), which describes six test problems used in the verification of GEOETHER. Of these six problems, analytical solutions were available for only one problem and portions of another. The remaining problems were used for intercode comparisons only. The problems for which analytical solutions were available are listed below:

1. Radial, steady state flow and unsteady heat transport in a single-phase liquid.
2. One-dimensional radial flow to a line sink (zero radius well) in a homogeneous porous medium. Case a involves a single-phase liquid, and case b a two-phase mixture of liquid and vapor. In case c, the fluid changes from a compressed liquid to a two-phase mixture as a flash front propagates away from the well.

The results of comparing GEOTHER code calculations with the analytical results for the above two test problems were not reported in ONWI-434. Although the remaining four test problems listed in ONWI-434 were used for intercode comparisons, only the results for the two problems discussed below are reported in ONWI-434.

Stanford workshop problem 3 involved two-dimensional flow to a well in a fracture/block medium, where vertical flow is allowed in the porous block and radial flow occurs in the fracture. Darcy flow is assumed. Comparison with results from a Lawrence Berkeley Laboratory code (Faust et al., 1982) shows good agreement for pressure within the block medium. A small discrepancy between the two codes, which increases with simulation time, is indicated for the pressure calculations within the fracture.

Standard workshop problem 5 involved multiphase flow in a two-dimensional horizontal reservoir. Mass is produced at one point in the reservoir, and recharge is induced over one of the lateral boundaries. In case "a," a fully penetrating production well is present. In case "b," a fully penetrating production well plus an injection well are present. All four codes used in the intercode comparisons showed similar results. Differences were attributed primarily to differences in the thermodynamic empirical expressions used in the sizes of the time steps used. However, there were insufficient results and discussion to demonstrate clearly that these were indeed the sources of differences and that they could not be attributed to problems with the codes themselves. For example, the authors should have performed sensitivity runs to demonstrate the sensitivity to time step size and accuracy of the thermodynamic expressions. It was noted in Stanford Geothermal Program (1980) that some of the tests were conducted with different versions of GEOTHER, but no detailed explanation was given. The reader is left with the feeling that the code verification effort has been wholly inadequate.

3.8.7 Validation

No validation exercises are reported in ONWI-434. A modified version of GEOTHER was used to "reproduce" steady state flow conditions at the Baca geothermal field in New Mexico (Faust et al., 1982). However, results are not given in the code documentation. Differences between this version and the code documented in ONWI-434 are not described. ONWI-434 also says that "the model [which version?] was also used in a sensitivity analysis to compare alternative proposed production schemes for the Baca field" (p. 52).^{*} ONWI-434 also notes that Faust and Mercer (1979a, b) describe a simulation of the Wairakei geothermal reservoir in New Zealand (p. 52). Again, no results are reported in ONWI-434.

3.8.8 Proposed ONWI Application

The GEOTHER code has not thus far been assigned any specific role in the assessment process by ONWI in available documents. ONWI-434 suggests that the code

^{*}Page numbers in Sec. 3.8 are from ONWI-434.

may have application in the near-field waste package environment where thermal loading may be important. However, ONWI-434 states that the likelihood of two-phase flow of pure water (or very dilute solutions) is unknown. The code could conceivably provide thermal input to a mechanical stress analysis code.

3.8.9 Relationship of Model to Other Codes

GEOETHER is a stand-alone code. It compliments other fluid and heat transport codes being considered by ONWI in that it treats two-phase flow of pure water. However, this additional capability is of limited applicability for the types of waste repository systems under consideration. The code could be used as a link between a thermal source term code like WAPPA and a mechanical stress analysis code.

3.8.10 Application of Code to Other Problems

The code was designed for application to geothermal reservoirs. See Sec. 3.8.7 for comments regarding code applications and references.

3.8.11 Suitability of Model for Salt Repository Application

It is not clear whether two-phase flow is likely to occur in a salt repository in the vicinity of the waste package. If it does, GEOETHER is the only code listed by ONWI that is capable of handling such flows along with heat transport. However, the code's application will be severely limited in that it has no provision for handling multicomponent solutions. The thermodynamic relations are only specified for mixtures of pure water in the liquid and vapor states.

3.8.12 Peer Review

No external peer review has been documented.

3.8.13 References for Section 3.8

Faust, C.R., and J.W. Mercer, *Geothermal Reservoir Simulation, 1: Mathematical Models for Liquid- and Vapor-Dominated Hydrothermal Systems*, Water Resources Research, 15(1):23-30 (1979a).

Faust, C.R., and J.W. Mercer, *Geothermal Reservoir Simulation, 2: Numerical Solution Techniques for Liquid- and Vapor-Dominated Hydrothermal Systems*, Water Resources Research, 15(1):31-46 (1979b).

Faust, C.R., et al., *Quantitative Assessment of Geothermal Development in the Lemez Mountains*, prepared by GeoTrans, Inc., Reston, Va., for the Bureau of Indian Affairs, Albuquerque, N.M. (1982).

INTERA Environmental Consultants, Inc., *GEOTHER: A Two-Phase Fluid Flow and Heat Transport Code*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-434 (April 1983).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

Stanford Geothermal Program, *Proc. Special Panel on Geothermal Model Intercomparison Study*, prepared for the U.S. Department of Energy, SGP-TR-42 (1980).

3.9 GRESS: GRADIENT-ENHANCED SOFTWARE SYSTEM

3.9.1 Code Description

GRESS (Oblow, no date, ORNL/TM-8339) is not a computer code for a model specifically designed for performance assessment of the waste package, repository, or a particular site. It is a general software package that could be used as a tool to facilitate sensitivity studies with model codes. However, the user's guide for GRESS simply describes the general package and does not discuss sensitivity studies for model codes as part of performance assessment. Thus, apart from the following brief summary of the package, no code summary is provided in this report.

GRESS is a FORTRAN compiler language that enhances conventional FORTRAN programs with analytic differentiation of arithmetic statements. It handles any standard FORTRAN code that contains arithmetic text material as part of the source program. The GRESS compiler reads the FORTRAN source code text, redefines the variables and their storage locations, searches for arithmetic statements, translates the latter for gradient calculations, and then generates a new source program that now includes gradient capabilities in all arithmetic statements. In summary, GRESS allows any standard FORTRAN code to be upgraded to calculate any derivatives required, whether they be for internal use in a calculation (e.g., for iteration) or for external use (e.g., sensitivity studies).

3.9.2 Reference for Section 3.9

Oblow, E.B., *GRESS: Gradient-Enhanced Software System, Version B, User's Manual*, Oak Ridge National Laboratory Report ORNL/TM-8339 (no date).

3.10 HEATING6: A MULTIDIMENSIONAL HEAT CONDUCTION ANALYSIS WITH A FINITE-DIFFERENCE FORMULATION

3.10.1 Code Description

The HEATING6 code is the most recent version of the HEATING (heat engineering and transfer in nine geometries) program. HEATING6 was developed from HEATING5 by (1) adding a free-form input package, (2) inserting more diagnostic messages, (3) putting in a thin surface boundary condition capability, and (4) refining the implicit numerical techniques used to solve the heat-balance equation.

HEATING6 solves steady state and transient heat conduction problems in one-, two-, or three-dimensional Cartesian coordinates; in one-, two-, or three-dimensional cylindrical coordinates; or in one-dimensional (radial) spherical coordinates. Thermal conductivity can be anisotropic and can depend on both spatial coordinates and temperature. Density and specific heat can, likewise, depend on both spatial coordinates and temperature. The heat generation rate per unit volume can be a function of time, position, and temperature. Materials can experience a change of phase. HEATING6 can treat problems whose boundary conditions depend on time and position. Boundary conditions can be in the form of specified temperatures or any combination of specified heat flux, forced or natural convection, and radiation. Also, it is possible to specify radiative heat transfer across regions embedded in the physical system being simulated.

Input to HEATING6 consists of system geometry, materials, a heat source function, initial temperatures, and boundary conditions. Output includes predicted temperatures. Output is obtained from input by solving a finite-difference formulation of the heat-balance equation. Steady state problems are solved by the point successive overrelaxation iterative method plus a modification of the "Aitken δ extrapolation process," with the direct solution technique being an alternative method when the problems are one- or two-dimensional.

Transient thermal transport problems can be solved by the implicit technique, by an explicit method that is stable for a time step of any size, or by the stability-limited classical explicit procedure. Of these three alternatives, the generally recommended method is the implicit technique, which ranges from the Crank-Nicolson procedure to the classical implicit procedure. The equations used in the implicit technique are solved by point successive overrelaxation iteration.

HEATING6 is quite generally formulated and appears to have only three limitations. First, when spherical coordinates are used, only the radial dimension is available. In contrast, with both Cartesian and cylindrical coordinates, all three dimensions are available. Second, HEATING6 includes only conductive heat transfer, not convective or radiative. This limitation could be overcome in the case of conductive and radiative heat transfer by using an effective thermal conductivity that includes the radiative contribution, provided the radiative absorption length is small compared to other scales of the system. Third, boundaries must be parallel to coordinate planes.

In the case of steady state problems, the user of HEATING6 should vary the mesh spacing and change the convergence criterion so as to develop confidence in the solution. These same steps should also be taken in the case of transient problems, but the user should also vary the time increment to be sure that the numerical solution has converged to the true solution.

HEATING6 is written in FORTRAN-IV (enhanced) for use on an IBM 3033 or 36-195 computer.

3.10.2 Development Stage

HEATING6 is complete and ready for use.

3.10.3 Documentation

HEATING6 is well documented in Elrod et al. (1981). However, the documentation departs from the NUREG-0856 (Silling, 1983) format in several respects.

1. A standard software summary is not included.
2. A section explicitly devoted to the presentation and discussion of the assumptions and limitations of the code is missing.
3. Model review is not discussed.
4. Code verification and model validation are not discussed.
5. Descriptions of the maintenance and quality assurance programs for the code are not provided.
6. Although Elrod et al. (1981) does not contain a separate section with the title "User's Manual," the information that should be presented in a user's manual is, in fact, thoroughly presented in the document.

3.10.4 Performance Specification Review

Performance specification review has only been done internally by Oak Ridge National Laboratory.

3.10.5 Code Design Review

Code design review has only been done internally by Oak Ridge National Laboratory.

3.10.6 Verification

Verification tests of HEATING6 are not described in Elrod et al. (1981) or in any other known document.

3.10.7 Validation

Validation tests of HEATING6 are not described in Elrod et al. (1981) or in any other known document.

3.10.8 Proposed ONWI Application

HEATING6 can be used for waste package and repository assessment. It is similar to DOT, except that DOT is limited to two dimensions. In repository assessment, HEATING6 has far greater general capabilities than TEMP and SALT4.

3.10.9 Relationship of Model to Other Codes

With respect to the other ONWI codes, HEATING6 is a stand-alone code. However, within the ORNL SCALE (standardized analyses for licensing evaluation of nuclear systems) system, it is an interactive code. Heating is very similar, but not identical, to the code THAC-SIP-3D as documented in Turner (1978).

3.10.10 Application of Code to Other Problems

HEATING6 was designed to solve heat flow problems arising in nuclear licensing applications.

3.10.11 Suitability of Model for Salt Repository Application

If there were significant convective heat transport in salt due to, say, water, then HEATING6 would not yield accurate results. If the radiative transfer in salt (salt is transparent in the infrared) were significant and if the radiative heat flow were not combined into an "effective" (conductive plus radiative) conductivity, then, again, HEATING6 would be inaccurate.

3.10.12 Peer Review

HEATING6 has not been subjected to peer review.

3.10.13 References for Section 3.10

Elrod, D.C., et al., *HEATING6: A Multidimensional Heat Conduction Analysis with the Finite Difference Formulation*, U.S. Nuclear Regulatory Commission Report NUREG/CR-0200, Oak Ridge National Laboratory Report ORNL/NUREG/SCD-2/V2, Vol. 2, Sec. F10 (Oct. 1981).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

Turner, W.D., *THAC-SIP-3D: A Three-Dimensional, Transient Heat Analysis Code Using the Strongly Implicit Procedure*, Oak Ridge Gaseous Diffusion Plant, Oak Ridge, Tenn., K/CSD/TM-24 (Sept. 1978).

3.11 LAYFLO: A ONE-DIMENSIONAL SEMIANALYTICAL MODEL FOR THE MIGRATION OF A THREE-MEMBER DECAY CHAIN IN A MULTILAYERED GEOLOGIC MEDIUM

3.11.1 Code Description

LAYFLO (Gureghian and Jansen, 1983, ONWI-466) calculates the transport of radionuclides in groundwater for site subsystem assessments where a layered geologic medium is present. The model output of concentration of radionuclides in groundwater (activity per unit volume) at some distance from a source can be used as input to biosphere dose codes.

LAYFLO solves a one-dimensional equation for the transport, dispersion, decay, and sorption-desorption of radionuclides in a multilayered geologic medium. For the fully dispersive case, up to six layers, each with a different constant value for bulk soil density, porosity, and dispersion coefficient, are permitted. For the nondispersive case (zero longitudinal dispersion coefficient), any number of layers is permitted. Sorption-desorption of radionuclides is represented by linear relationships as the products of radionuclide concentrations and distribution coefficients, which can take on different constant values for each layer. Consequently, retardation factors (distribution coefficients combined with soil density and porosity) may have different constant values in each layer.

First-order radioactive decay is specified for three-membered decay chains. The source of radionuclides at the beginning of the flow path can take one of two forms: a continuous source that changes with time in accord with radioactive decay, or a band release for which concentrations become zero after some given finite time interval.

The model is applied in the following manner. A multilayered geologic medium of distinct layers is subjected to fully saturated groundwater flow. The results from another model or analysis of this flow system delineates streamtubes (stream lines in two dimensions) through which flows groundwater at a constant rate. The one-dimensional

model LAYFLO is assumed to apply through such a streamtube, which contains distinct layers, each having different, but constant, velocities, hydraulic properties, and sorptive properties. Given these properties, the source type and concentration, and the radionuclide decay constants for the three-member chain, LAYFLO predicts the concentration (activity per unit volume) of each radionuclide as a function of time and distance from the source.

The solution technique for LAYFLO is semianalytical in that the governing equations, source terms, and boundary conditions, including those between adjacent layers, are subjected to Laplace transforms, and the convolution theorems used to obtain inverse Laplace transforms result in expressions requiring numerical solution. In particular, summations and integrals involving exponential and complimentary error functions are required. Gauss-Legendre quadrature and various approximations and asymptotic expansions are used. Complications in the evaluation of some terms require iteration and, if the complications are not resolved successfully after two iterations for the dispersive case, the nondispersive solution is sought.

The code has been run on the CDC CYBER 74 using FORTRAN IV. There are 3280 source program statements, and the storage requirements are 133,200 octal words (Gureghian and Jansen, 1983). The graphics package used with LAYFLO is apparently DISSPLA.

Several underlying assumptions and limitations need to be considered in applying LAYFLO. Groundwater flow must be fully saturated and steady. Transverse dispersion of the contaminant is neglected by the one-dimensional nature of the model. The assumption of distinct layers and uniformity within each layer usually represents a simplification of actual geologic conditions. Implicit in the model formulation is the assumption that the flow field is not modified by heat generation or by the chemical composition of the water as it might affect viscosity and density. Dissolution of salt might, for example, violate this assumption.

3.11.2 Development Stage

The model as described in ONWI-466 was developed recently and has undergone some testing by its developers. It has apparently been made available to the National Energy Software Center. It is not fully documented in ONWI-466; documentation of use by others is not available.

3.11.3 Documentation

LAYFLO is not documented in ONWI-466 as suggested in NUREG-0856 (Silling, 1983), and it would be nearly impossible to run LAYFLO on the basis of the information provided in ONWI-466. While a theoretical basis for the model, along with the governing equations, is given, and several verification tests are described very briefly, the actual numerical solution technique and computer code are not discussed in any detail. Some portions of the analytical solution development are difficult to follow because of undefined notation and limited text explanation. There is neither a user's manual nor a

listing of the code in ONWI-466. The single-solution flowchart and two appendixes related to numerical evaluations of portions of the equations are inadequate for detailed understanding of the solution procedure.

Discussions of model assumptions, limitations, solution stability and accuracy, and code support and maintenance procedures are insufficient to satisfy NUREG-0856 requirements. Although the abstract and the standard software summary in ONWI-466 point out that the dispersive case is limited to consideration of six layers, that limitation is not mentioned in the text. Moreover, solutions for the dispersive case are carried out in the text for the n th layer, with no discussion of the reason for the limitation to six layers in computation.

3.11.4 Performance Specification Review

There is no documented evidence of performance specification review other than what has been conducted by the code developers.

3.11.5 Code Design Review

The only evidence of code design review is the statement that the National Energy Software Center has tested the code. However, the results of those tests are not presented.

3.11.6 Verification

Several verification tests of parts of the model and the entire model are reported briefly. These tests and the results can be summarized as follows:

1. Two- and Three-Layered Medium, No Sorption, No Decay. Predictions were made to investigate the response of (and in a sense to validate) the transport and dispersion portions of the solution without sorption or decay. (It is not clear whether the full code was run with those parameters at zero or whether a separate analytical solution was constructed.) The predictions were for two- and three-layered systems in sand, for which Shamir and Harleman (1966) had laboratory experimental data. The agreement with the results of these short-time experiments is relatively good, with some deviations between predictions and data in the later part of the breakthrough curves.
2. Homogeneous (one-layered) Medium, Nondispersive. The case of $^{234}\text{U} + ^{230}\text{Th} + ^{226}\text{Ra}$ was examined for the radionuclide and hydrologic conditions set forth in case 1.3 INTRACON (Grundfelt and Anderson, 1983) and compared with the results of code UCB-NE-25. Excellent agreement was found. Comparisons of two

slightly dispersive (large Peclet numbers -- 5×10^3 and 5×10^4) runs showed close agreement with each other for ^{230}Th . However, the large Peclet number cases produced ^{230}Th concentrations almost double those of the nondispersive solution. The unexpected increase in concentration with the addition of dispersion runs, which is counter to physical intuition, is not discussed.

3. Homogeneous (one-layered) Medium, Dispersive. The case of $^{234}\text{U} \rightarrow ^{230}\text{Th} \rightarrow ^{226}\text{Ra}$ was examined for the radionuclide and hydrologic conditions set forth in case 1.33 INTRACOIN (Grundfelt and Anderson, 1983), which is the same as case 1.3 except for higher dispersion. The results were compared with those resulting from using code UCB-NE-10.2. Excellent agreement was found. The Peclet number for this dispersive case was 10 (relatively high dispersion). The results for ^{230}Th concentrations in this case are almost identical to those of the nondispersive case. This unexpected result, that is, almost no dispersion effect, has not been explained or discussed.
4. Two-Layered Medium, Nondispersive. The cases of $^{234}\text{U} \rightarrow ^{230}\text{Th} \rightarrow ^{226}\text{Ra}$ and $^{245}\text{Cm} \rightarrow ^{237}\text{Np} \rightarrow ^{233}\text{U}$ were examined for the conditions of cases 2.1 and 2.3 INTRACOIN (Grundfelt and Anderson, 1983), respectively. The results of LAYFLO and code UCB-NE-30 agreed exactly for these cases.
5. Three-Layered Medium, Dispersive. Three cases were investigated using the decay chains used in the two-layered case, a dispersive Peclet number of 10, and two different sets of retardation coefficients. The results of LAYFLO were compared with several INTRACOIN results (Grundfelt and Anderson, 1983), and fair agreement was noted in the majority of solutions. The descriptions and identification of the solutions to which the LAYFLO results were compared were inadequate to allow any general conclusions to be reached.

3.11.7 Validation

With the exception of the no-sorption and no-decay case comparisons mentioned in ONWI-466, no validation studies have been reported.

3.11.8 Proposed ONWI Application

The proposed application of LAYFLO appears to be for performance assessment at site scale in cases where a layered medium exists. The area of application would need to be sufficiently far from the repository so that heat generation would not be an

important process. The groundwater flow pattern through the layered medium would have to be determined prior to application of LAYFLO, as would the source terms.

The code SWENT might, in theory, handle the case of a multilayered geologic medium in its prediction of groundwater flow, energy transfer, and radionuclide transport. However, LAYFLO is simpler to operate, as it predicts only radionuclide transport.

3.11.9 Relationship of Model to Other Codes

LAYFLO does not require direct input from other codes. However, the groundwater flow-field parameters required as inputs for LAYFLO could be derived from groundwater flow models. Specification of the radionuclide source terms could come from a repository assessment model, or the terms could be specified independently. The output of LAYFLO nuclide concentrations in a given groundwater flow provides the release rates required as input to the biosphere transport and dose assessment codes, PABLM and DACRIN.

LAYFLO appears to be an extension of GETOUT, a one-dimensional code for single-layer radionuclide transport based on a Laplace transform solution.

3.11.10 Application of Code to Other Problems

No applications of the LAYFLO code to other problems are documented.

3.11.11 Suitability of Model for Salt Repository Application

Dissolution of salt in domes or bedded formations could violate several important assumptions underlying LAYFLO. Concentrations of solutes are not permitted to modify flow properties like viscosity or density, which could in turn modify the flow field. Also, in the case of significant dissolution, sorption characteristics might vary substantially through the medium.

3.11.12 Peer Review

No peer or independent review of LAYFLO is documented.

3.11.13 References for Section 3.11

Grundfelt, B., and K. Anderson, *INTRACON — Report of Final Results of Level 1, International Nuclide Transport Code Intercomparison Study* (1983).

Gureghian, A.B., and G. Jansen, *LAYFLO: A One-Dimensional Semianalytical Model for the Migration of a Three-Member Decay Chain in a Multilayered Geologic Medium*, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-466 (1983).

Shamir, U.Y., and D.R.F. Harleman, *Numerical and Analytical Solutions of Dispersion Problems in Homogeneous and Layered Aquifers*, Massachusetts Institute of Technology Report No. 89, Cambridge, Mass. (1966).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

3.12 MMT: A RANDOM-WALK ONE-DIMENSIONAL MULTICOMPONENT MASS TRANSPORT CODE

3.12.1 Code Description

The MMT code (INTERA, 1983, ONWI-432) calculates the transport of radionuclides in groundwater. Its output of radionuclide release rates as a function of time at the end of the specified flow path is appropriate input to biosphere dose codes for site assessment.

The MMT code solves a one-dimensional equation for the transport, dispersion decay, and sorption-desorption of radionuclides in a simplified groundwater system. The groundwater system is characterized by constant (spatially uniform and steady) velocity, constant porosity, constant bulk density, and a constant longitudinal dispersion coefficient. The sorption-desorption of radionuclides is represented in the model by a linear relationship as the products of radionuclide concentrations and spatially uniform distribution coefficients. The distribution coefficients and related retardation coefficients depend on bulk rock properties and average geochemical data and must be specified as input to the model.

Radioactive decay of up to 10 different radionuclides can be accommodated. First-order radioactive decay can be included, as can linear or branched decay chains (with daughter products) with an arbitrary number of members. Specification of the source of radionuclides for the one-dimensional framework is relatively general. The source can have a general time dependence; that is, it does not have to be restricted to an impulse or band release. For example, the release can be "leach-limited," with an arbitrary form of leach rate, or it can be "solubility-limited," with a constant concentration but variable mass.

A simplified summary of the input to the code follows. The groundwater system is characterized by its transport velocity, dispersion coefficient, bulk density, and porosity. The height, width, and length of the "one-dimensional" transport pathway are specified. Each radionuclide contaminant is identified by a code number relating it to an external library of half-life data, is assigned a distribution coefficient for sorption-desorption, and is given an initial inventory in curies. Radioactive decay is specified as no chain, linear chain, or branched chain, and decay constants must be entered. The source of radionuclides is described both spatially and in time in terms of (1) the center of the release position along the direction of flow, (2) the length of the initial release

position, (3) the time of the start of leaching, (4) the fraction-of-inventory-remaining versus time function, and (5) the total time of leaching.

Given these input data, the code accounts for transport, dispersion, sorption-desorption, and radioactive decay, as the contaminants are carried away from the source region. The release rate in curies per year is calculated for each individual contaminant at the end of the specified flow path as a function of time.

The numerical solution of the governing equation follows a discrete-parcel-random-walk (DPRW) approach in contrast to a finite-difference approach. The DPRW approach is inherently stable and minimizes computational errors associated with finite-difference solutions to problems with a convective transport component. Such errors are often manifested by difficulties in conserving mass. While there is some numerical dispersion in the DPRW approach resulting from generation of members of a decay chain with different retarded transport velocities, the dispersive error does not accumulate to frustrate mass conservation.

The DPRW simulation traces the behavior of a finite number of discrete parcels through the system. There is no means of determining the number of parcels and the accuracy of the results other than by experience and solution comparisons. The DPRW solution usually takes more computational time than comparable finite-difference solutions for which stability and accuracy are acceptable, but, for many problems, the inherent stability and accuracy of DPRW offset the increased time requirements. Solution accuracy increases as the square root of the number of parcels used, and in the case of linear source terms, solutions from independent computations can be averaged to increase accuracy. A certain amount of statistical noise in the solutions results from the random-walk aspect of the simulation. Postprocessing with a variable-window, moving-average filtering method is available to deal with this problem.

The computer program compiles on a FTN5 compiler for CDC systems, particularly the CYBER 176. The compiler is compatible with the FORTRAN V language. The program is set up for mixed batch and interactive usage. The interactive aspect facilitates setting up the problem to be run, whereas the production of raw nuclide release rates is done in batch mode. A plotting routine compatible with CALCOMP software is used. The core storage requirement is largest for the main release rate computation, which requires approximately 77,000 decimal words.

There are several general assumptions and limitations of MMT that should be considered before application. The groundwater transport system is highly simplified: fully saturated flow and temporal and spatial uniformity are assumed. Consideration of dispersion is limited to the longitudinal direction because of the one-dimensionality, which means that transverse dispersion is neglected. The flow field is assumed to be independent of the temperature and chemical composition of the groundwater. Thus, flow fields affected by heat sources cannot be handled by this approach. Also, significant dissolution of the porous medium (particularly salt) would invalidate the MMT approach.

3.12.2 Development Stage

The version of MMT described in INTERA (1983) was modified by INTERA in 1983 for use on CDC computer systems. The theoretical and numerical approaches for MMT were established earlier at Battelle's Pacific Northwest Laboratories (Ahlstron et al., 1977; Washburn et al., 1980). INTERA has also initiated verification of MMT.

3.12.3 Documentation

The MMT code is documented in ONWI-432 in accordance with the guidelines of NUREG-0856 (Silling, 1983), including a complete user's manual and program listing.

3.12.4 Performance Specification Review

The only documented performance specification review is the one in ONWI-432. No peer review or other outside review of MMT has been documented.

3.12.5 Code Design Review

Preparation of ONWI-432 constitutes the only documented code design review. While a "reader's comments" card is provided in ONWI-432 for comments on code performance, no outside code design reviews have been documented.

3.12.6 Verification

Comparisons of the results of MMT and existing analytical solutions for two different cases with the same hydrologic parameters are described in ONWI-432. One case considers the fate of a single radionuclide, ^{129}I , and the other of a two-member decay chain of ^{248}Cm and ^{244}Pu . The analytical solutions were from Lester et al. (1975). The hydrologic data were (1) groundwater velocity = 100 meters per year, (2) length of flow path = 10,000 meters, (3) bulk density of soil to porosity ratio = 5 grams per milliliter, and (4) longitudinal dispersion coefficient = 1 square meter per year. The nuclides were apparently released (leached) linearly from the source for 1000 years. The data on the nuclides for both cases are shown in Table 3.

Numerical solutions for MMT were found for a base case for ^{129}I , ^{248}Cm , and ^{244}Pu using parcel densities of 6500, 3250, and 7500, respectively. Then, for each nuclide, the corresponding particle densities were doubled, increased fourfold, and increased eightfold. For ^{129}I , increased parcel density resulted in increased agreement between numerical and analytical results, primarily in the timing of peak release rates. The same was true for ^{248}Cm . However, the release rate histories for the daughters of ^{248}Cm and ^{244}Pu showed shifts in peak locations with increasing parcel density. In all cases, agreement between MMT results and the analytical solutions was quite good, with deviations in release rates being less than 10%. INTERA felt that deviations from analytical results could be attributed to the statistical nature of MMT results and the

TABLE 3 Nuclide Data Used in Comparing MMT and Existing Analytical Solution Results

Nuclide	Inventory (curies)	Half-Life ^a (yr)	Distribution Coefficient (mL/g)	Retardation Coefficient
¹²⁹ I	1.0	1.72×10^7	0	1
²⁴⁸ Cm	0.5	4.7×10^5	333	1666
²⁴⁴ Pu	5.36×10^{-5}	7.6×10^7	1000	5001

^aThese half-life values are incorrect but were used consistently in both the MMT and analytical solutions.

Source: INTERA (1983).

smoothing filter. Also, the finite length of the path for MMT, in contrast to the infinite boundary conditions for the analytical solution, may have affected the comparisons.

3.12.7 Validation

No validation studies with MMT have been found. According to ONWI-432, no formal validation has been performed.

3.12.8 Proposed ONWI Application

ONWI proposes to use MMT for performance assessment in the far field. It is anticipated that MMT can be used where the one-dimensional simplification of the groundwater system can be justified (perhaps as the result of more detailed groundwater system study) and where the distance from the repository will permit neglecting temperature influences on the flow field. The generalized form of the radionuclide source terms and the flexibility of handling several nuclides with branched decay chains makes MMT attractive for screening the relative merits of various proposed or hypothetical waste disposal systems. The simplified nature of the hydrologic environment representation may mean that MMT will have greater value for such screening than it will for detailed analysis of a specific site.

Two other codes address generally similar problems. The SWENT code evaluates hydrologic flow and energy transfer, as well as radionuclide transport. Because it handles the coupling among these processes, it is much more sophisticated. However, numerical dispersion presents a problem because SWENT has a finite-difference solution. MMT has the flow field specified and uncoupled from energy and radionuclide transport;

therefore, it is far simpler to apply than SWENT. GETOUT is similar to MMT in that it is one dimensional, with constant transport properties. GETOUT has a Laplace transform solution approach that limits the application to three-member decay chains and to impulse or fixed-band source terms. Being less limited, MMT is more versatile than GETOUT.

3.12.9 Relationship of Model to Other Codes

The MMT code does not require direct input from other codes. However, the groundwater flow field required as input could be derived from groundwater flow models. Radionuclide source terms could be specified using results from repository assessment models or could be specified independently. MMT does require input on radionuclide half-lives from the data library SWNUCLB, a radionuclide library that is part of the INTERA SCEPTER program.

The output of MMT -- radionuclide release rates as a function of time at the end of the flow path -- can be used directly as input to a biosphere transport and dose assessment code like PABLM.

3.12.10 Application of Code to Other Problems

As stated in ONWI-432, MMT has been applied to a number of problems. However, no documented applications have been cited.

3.12.11 Suitability of Model for Salt Repository Application

The major difficulty in applying MMT to sites in salt domes or bedded salt formations is the assumption that concentrations of solutes in the groundwater are so low that they do not affect the viscosity or density of the solution significantly. Violation of this assumption with regard to either parameter could result in serious modifications to the transport flow field. Also, if dissolution is significant, there is the possibility of major changes in the sorption-desorption characteristics of the medium.

3.12.12 Peer Review

No independent review of MMT has been documented.

3.12.13 References for Section 3.12

Ahlstron, S.W., et al., *Multicomponent Mass Transport Model: Theory and Numerical Implementation (Discrete-Parcel-Random-Walk Version)*, Battelle Pacific Northwest Laboratories, Richland, Wash., BNWL-2127 (1977).

INTERA Environmental Consultants, Inc., *MMT: A Random-Walk One-Dimensional Multicomponent Mass Transport Code*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-432 (April 1983).

Lester, D.H., et al., *Migration of Radionuclide Chains through an Adsorbing Medium*, Adsorption and Ion Exchange, American Institute of Chemical Engineers Symposium Series 152, 72:202-213 (1975).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

Washburn, J.F., et al., *Multicomponent Mass Transport Model: A Model for Simulating Migration of Radionuclides in Ground Water*, Battelle Pacific Northwest Laboratories, Richland, Wash., PNL-3179 (1980).

3.13 NETFLO: A NETWORK GROUNDWATER FLOW CODE

3.13.1 Code Description

NETFLO (INTERA, 1983, ONWI-425) represents three-dimensional, steady state, fully saturated groundwater flow in a heterogeneous medium as flow through an equivalent network of pipes in series and in parallel. The pipes are connected at nodes. The equivalent network must be indicated by the stratigraphy of the geologic system being modeled or must be suggested by stream tubes that are identified by using a more detailed, three-dimensional code to simulate the geologic system. The "correct" network (i.e., one with the correct pipe locations, orientations, lengths, diameters, and permeabilities) is one that, for all plausible boundary conditions, provides the same output as a more detailed, three-dimensional, verified and validated code. Of course, if one has to determine "correctness" by comparison with a more detailed model and do it over a full range of boundary conditions, there is no advantage to be gained in using NETFLO. If, for a given network, NETFLO agrees with a more detailed code for just one set (or a few sets) of boundary conditions, then one assumes that it will agree for all such conditions, making it the "correct" network. This "leap of faith" is the basic assumption in NETFLO.

Input to NETFLO consists of the lengths and cross-sectional areas of the pipes, the permeability and porosity of the porous medium in the pipes, the density and viscosity of the water flowing through the pipes, the elevations of the nodes, and the pressure or flux boundary conditions. These conditions specify either the pressure on a boundary or the flux of water into or out of various nodes. Output consists of the pressures at all nodes plus water velocity and flow rate in each pipe.

The output is obtained from the input by solving two basic equations: an equation that expresses the conservation of mass at each node and the Darcy equation for fluid flow through a porous medium. These equations are combined at each node, and

the resulting set of N equations for N nodes is cast into the form of a single matrix equation. The N equations are solved by Gaussian elimination.

The limitations of NETFLO are: (1) the network representation for a given geologic site must be verified by comparing NETFLO's output with that of a more rigorous model, such as SWENT or FE3DGW; (2) one needs to make the "leap of faith" mentioned above; (3) when NETFLO is combined with the codes GETOUT and PABLM in an integrated package, the limitations of these latter two codes also apply to NETFLO; and (4) NETFLO does not take into account the absorption of water in salt or changes in the permeability of fractured (or porous) salt resulting from the dissolution of salt in the flowing groundwater.

The NETFLO code requires little computer time compared with a more rigorous, three-dimensional finite-difference or finite-element code. For this reason, it appears to be well suited for sensitivity analysis. NETFLO is written in FORTRAN IV for use on a CDC CYBER 176 computer.

3.13.2 Development Stage

NETFLO is fully developed and ready for use.

3.13.3 Documentation

NETFLO is well documented in ONWI-425 and follows the NUREG-0856 (Silling, 1983) guidelines. The NETFLO documentation should, however, be improved by making the following, generally minor, changes:

1. The water density, ρ , is presented as a subscripted variable, implying that it may vary from one pipe to the next. But, no equation is given to describe ρ as a function of pressure. Hence, the water is presumably being taken to be incompressible. If so, there is no need to present ρ as a subscripted variable (p. 7).*
2. The text should point out that for flow through porous or fractured salt, NETFLO does not take into account the interaction of the water with the salt (p. 8).
3. The documentation should present at least two examples of the type of sensitivity analysis that is NETFLO's forte. What are the variables, for example, whose effect on the output one wishes to determine in a sensitivity analysis? Given that a more exact code (e.g., SWENT or FE3DGW) is needed to accomplish "preliminary verification over a range of parameters for a specific site," the statement that NETFLO is relatively economical needs to be justified (p. 8).

*Page numbers in Sec. 3.13 are from ONWI-425.

4. The word "output" should be replaced in the table by the word "dimensions" (p. 9).
5. The "=" sign is missing in Eq. 3-1 (p. 15).
6. There is no Fig. 3-6 (p. 16).
7. "Gaussian elimination" should be briefly described (p. 17).
8. An example of, say, a three-node system should be presented and the equations put in matrix form, with the types of boundary conditions illustrated (pp. 6-17).
9. At the bottom of page 19, the absolute value signs are omitted.
10. The reference to "the repository node" implies that, when NETFLO is used for nuclide transport calculations, the repository is represented as a single node. If so, this should be stated explicitly (p. 20).
11. Replace "Eq. 10" with "Eq. 7" (p. 20).

3.13.4 Performance Specification Review

An internal performance specification review by INTERA and ONWI has been completed. No external performance specification review has been conducted.

3.13.5 Code Design Review

An internal code design review by INTERA and ONWI has been completed. There has been no external code design review.

3.13.6 Verification

The NETFLO code was used to solve two two-dimensional example problems that had been solved previously by Sandia National Laboratories' network model (Campbell et al., 1980). According to ONWI-425, there was perfect agreement between the NETFLO solution and the Sandia solution for each of the example problems. However, only the NETFLO solution is presented in ONWI-425. Because the two example problems were quite similar, they should not be considered to be fully independent verifications.

The NETFLO code was also used to solve an electrical network current-flow problem, with the solution compared with the analytic solution. The two solutions are displayed in ONWI-425 and are identical. NETFLO should be verified in a greater variety of cases than the three reported in ONWI-425.

3.13.7 Validation

As with any code that models physical systems, the procedure for validating NETFLO is to compare its predictions of behavior of various physical systems with the observed behavior of those systems. As a kind of surrogate validation, NETFLO predictions could be compared with those of another model that has been thoroughly verified and validated. NETFLO has not yet been validated in either sense.

3.13.8 Proposed ONWI Application

The NETFLO code is intended for both repository and site subsystem assessment.

3.13.9 Relationship of Model to Other Codes

The NETFLO code provides input to the code GETOUT which, in turn, provides input to PABLM. GETOUT simulates nuclide transport in the geosphere, while PABLM determines the radiological dose to man.

3.13.10 Application of Code to Other Problems

No other application of NETFLO is known.

3.13.11 Suitability of Model for Salt Repository Application

The NETFLO code is suitable for modeling the flow of groundwater to and from a salt formation. It is, however, not suitable for modeling water flow within a salt formation, because it does not account for absorption of water into salt or for dissolution of salt into the flowing water.

3.13.12 Peer Review

No special peer review of NETFLO is planned by ONWI.

3.13.13 References for Section 3.13

Campbell, J.E., et al., *Risk Methodology for Geologic Disposal of Radioactive Waste: The Network Flow and Transport Model*, Sandia National Laboratories Report SANDIA-1920 and U.S. Nuclear Regulatory Commission Report NUREG/CR-1190 (1980).

INTERA Environmental Consultants, Inc., *NETFLO: A Network Ground-Water Flow Code*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-425 (1983).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

3.14 ORIGEN2: A REVISED AND UPDATED VERSION OF THE OAK RIDGE ISOTOPE GENERATION AND DEPLETION CODE

3.14.1 Code Description

ORIGEN2 (Croff, 1980a, ORNL-4628) is a point depletion and decay computer code for simulating nuclear fuel cycles and calculating the nuclide compositions of materials associated with the nuclear fuel cycle. The code is an updated version of the ORIGEN code that was distributed by Oak Ridge National Laboratory (Bell, 1973). It can be applied to a wide variety of fuel cycle flow sheets and fuel/reactor-type combinations. The code generates, as a function of time after irradiation, spent fuel and waste characteristics, including nuclide inventory, radioactivity, and thermal power. This information is needed for design of fuel reprocessing plants, spent fuel and waste shipping casks, and waste treatment and disposal facilities. Outputs also include radioactive ingestion and inhalation toxicity, and chemical ingestion toxicity. In other words, the code calculates the amount of air or water required to dilute substances to acceptable levels.

The buildup and depletion of nuclides in materials during irradiation are calculated using point geometry and quasi-one-group neutron cross sections. The model does not account for spatial or resonance self-shielding effects or changes in the neutron spectrum other than those encoded initially. However, provision is made to incorporate appropriate cross sections from more sophisticated reactor physics codes. This option requires calculations using separate codes supplied by the user.

The buildup and depletion processes are represented by a system of first-order ordinary differential equations with constant coefficients. This system is solved using a matrix exponential numerical method that is so memory intensive that a recursion relation is used to reduce the memory requirements. To maintain numerical accuracy and keep computing time down, only the long-lived isotopes are treated with the matrix exponential method. Alternative techniques are used for the short-lived isotopes.

ORIGEN2 requires three data libraries that can be prepared from three master libraries at Oak Ridge National Laboratory by its staff. User-supplied input data are also required. Cross sections from other, more sophisticated reactor physics codes may also be required if the point geometry assumptions used in ORIGEN2 are inadequate.

The code is composed of some 60 subroutines. An overlay procedure is used to conserve core memory space. Written entirely in FORTRAN, the code is composed of some 7300 source statements. Versions are available through Oak Ridge National Laboratory's Radiation Shielding Information Center for both IBM and CDC machines. Core requirements range from 175K to 600K, depending on the problem size.

3.14.2 Development Stage

The ORIGEN2 code is a substantially revised version of the ORIGEN code that has been in use since the late 1960s and early 1970s.

3.14.3 Documentation

The documentation does not conform to NUREG-0856 (Silling, 1983). It includes a brief description of ORIGEN2 (Croff, 1980a), a technical description of the original ORIGEN code (Bell, 1973), and a user's manual for ORIGEN2 (Croff, 1980b). The documentation of ORIGEN2 in ORNL-4628 provides a brief description of the differences between ORIGEN2 and ORIGEN, but ORNL-4628 is not a stand-alone documentation of the ORIGEN2 code. Furthermore, a standard software summary is not included.

The user's manual is poorly written from the point of view of a new user. It does not describe what the code does or how it does it. There are no charts showing either the overall or the detailed structure of the code and no information about what the subroutines are and something of their function.

3.14.4 Performance Specification Review

No performance specification review of ORIGEN2 has been documented.

3.14.5 Code Design Review

No code design review of ORIGEN2 has been documented.

3.14.6 Verification

Code verification of ORIGEN2 has not been discussed in the available code documentation.

3.14.7 Validation

Validation exercises for ORIGEN2 have not been documented.

3.14.8 Proposed ONWI Application

ONWI does not indicate what specific problems require the use of ORIGEN2, except to say that it can be used for "waste package subsystem analyses." Because several other models have been selected for specific roles in the waste package assessment plan, it appears that ORIGEN2 could serve as the source-term generator for those other models. If so, it would be worthwhile to look into how well that role could be

satisfied by ORIGEN2 and, in particular, what modifications, if any, would be required to satisfy that role.

3.14.9 Relationship of Model to Other Codes

ORIGEN2 provides source-term information on the element and isotope inventories of the waste form, radiation levels, and heat generation as a function of time. This information is required by the process models contained in the WAPPA package, as well as by other codes used in performance assessment of the waste package and its immediate surroundings. However, the detailed links between ORIGEN2 and WAPPA, for example, are not discussed in the documentation, and it is not known if any additional data processing is required.

3.14.10 Application of Code to Other Problems

ORIGEN2 is a revision of ORIGEN, a code that has been widely distributed since the early 1970s. Although it has been used by Oak Ridge National Laboratory for license application calculations, specific applications of ORIGEN2 are not cited in the documentation.

3.14.11 Suitability of Model for Salt Repository Application

Because ORIGEN2 is a source-term code, its application to a specific type of repository is not at issue, so long as the waste form can be handled by the code. Details regarding the specific waste form and the ability of ORIGEN2 to handle such a waste form have not been documented.

3.14.12 Peer Review

The documentation does not indicate that ORIGEN2 has been peer reviewed.

3.14.13 References for Section 3.14

Bell, M.J., *ORIGEN — The ORNL Isotope Generation and Depletion Code*, Oak Ridge National Laboratory Report ORNL-4628 (May 1973).

Croff, A.G., *ORIGEN2 — A Revised and Updated Version of the Oak Ridge Isotope Generation and Depletion Code*, Oak Ridge National Laboratory Report ORNL-4628 (1980a).

Croff, A.G., *A User's Manual for the ORIGEN2 Computer Code*, Oak Ridge National Laboratory Report ORNL/TM-7175 (1980b).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

3.15 PABLM: A COMPUTER PROGRAM TO CALCULATE ACCUMULATED RADIATION DOSES FROM RADIONUCLIDES TRANSPORTED TO AQUATIC AND TERRESTRIAL PATHWAYS IN THE BIOSPHERE

3.15.1 Code Description

PABLM (INTERA, 1983, ONWI-446) is a biosphere transport and dose code for both acute and chronic exposures that calculates internal radiation doses to humans from ingestion of food and water contaminated with radionuclides and from external radiation doses from radionuclides in the environment. Radiation doses from radionuclides in the environment can be calculated from deposits on soil or plants during an atmospheric or liquid release, or from exposure to residual radionuclides after the releases have ended. Radioactive decay is considered during the release, after deposition, and during storage of food after harvest. The radiation dose models consider exposure to radionuclides (1) on the ground or on crops as a result of deposition from contaminated air or irrigation water, (2) in contaminated drinking water and in aquatic foods raised in contaminated water, and (3) in bodies of water and sediments where people might fish, boat, or swim. For vegetation, the radiation dose model considers both direct deposition and uptake through roots.

Doses can be calculated for either a maximally exposed individual or for a population group. The program can also calculate accumulated radiation doses from chronic ingestion of food products that contain radionuclides and from chronic external exposure to radionuclides in the environment. A first-year committed dose is calculated as well as an integrated dose for a selected number of years.

A chain decay scheme including branching for transitions to and from isomeric states is used for radioactive decay. The equations for calculating internal radiation doses are derived from those given by the International Commission on Radiological Protection (ICRP) for body burdens and the maximum possible concentration for each radionuclide (ICRP, 1959). These doses are calculated as a function of radionuclide concentrations in food products, ingestion rates, and radionuclide-specific dose-commitment factors. Radiation doses from external exposure to contaminated water and soil are calculated using the basic assumption that the contaminated medium is large enough to be considered an "infinite" volume or plane relative to the range of emitted radiation. The equations for calculating the radiation dose from external exposure to shoreline sediments include a correction for the finite width of the contaminated beach.

The code can accommodate no more than 23 possible body organs or tissues, 19 ingestion pathways, five organs and 100 radionuclides in a mixture, and four external exposure pathways.

The programming language is FORTRAN V. The computer for which the program was designed and other available machine version packages are the UNIVAC 1100 and CDC systems. Eighty thousand words of memory are required to execute the PABLM program. The National Energy Software Center (1981) reports executing sample problems in two minutes of CPU time on a UNIVAC 1100/44.

3.15.2 Development Stage

PABLM is ready for use. It is available in an operational UNIVAC, as well as in an operational CDC, version.

3.15.3 Documentation

The CDC version of PABLM is documented in NUREG-0856 format (Silling, 1983) in ONWI-446, which contains a federal information processing standard summary, a user's manual, and a sample case. The UNIVAC version is fully documented in Napier et al. (1980) and is further documented by the National Energy Software Center (1981). Additional summary documentation of PABLM is available in Science Applications (1981) and Shriner and Peck (1978). The documentation summary of PABLM in Science Applications (1981) is erroneous with respect to purpose, description, and keywords, in that it incorrectly identifies PABLM as a code dealing with ingestion of radionuclides from the air pathway.

3.15.4 Performance Specification Review

The UNIVAC version of PABLM has been accepted by the nuclear industry and NRC, and has been used extensively in the licensing of nuclear projects (U.S. Department of Energy, 1980; Office of Nuclear Waste Isolation, 1983). No performance specification review has been carried out specifically for nuclear waste isolation applications.

3.15.5 Code Design Review

The UNIVAC version of PABLM has been accepted by the nuclear industry and NRC, and has been used extensively in the licensing of nuclear projects (U.S. Department of Energy, 1980; Office of Nuclear Waste Isolation, 1983). No performance specification review has been carried out specifically for nuclear waste isolation applications.

3.15.6 Verification

The version of the PABLM code incorporated into the SCEPTER (Brecher and Pearson, 1983) package is reported in ONWI-446 as having been thoroughly checked to ensure that it produces results that are substantially the same as those from the earlier version of the code as documented in Napier et al. (1980). These efforts were designed to ensure that the modifications of the code to generalize its application to CDC and

other computer systems, and to provide integration with other codes in the SCEPTER package, did not lead to errors.

As a verification test, an aquatic release sample problem described in the documentation of the original code was checked. The sample problem calculates the dose to a maximally exposed individual living downstream from a groundwater discharge point. The groundwater is assumed to be contaminated with radionuclides and to be seeping into a river. (In the original application, this problem included a tank leaking radionuclides into a river. While it would be unlikely that this description would apply to a repository system, it was used for the sample case.)

The biosphere pathways in the above sample problem assume that the individual uses the contaminated river for irrigation water, fishing, and drinking water. Chronic exposure is assumed to occur over a 70-year period. Five radionuclides, ^3H , ^{14}C , ^{90}Sr , ^{137}Cs , and ^{239}Pu , are released to the river at time equals 1000 years, with initial release rates of 50, 5, 0.5, 1.0, and 0.1 Ci/year, respectively. The PABLM code automatically includes the important daughter products of the selected radionuclides in the evaluation. The results of running this sample problem with the new PABLM code were found to agree very well with those using the earlier version (Napier et al., 1980).

3.15.7 Validation

PABLM is based on the well-known ICRP-2 methodology, which has been used for many years. In addition, PABLM appears to have been accepted as valid for use by NRC and the nuclear industry, and has been used extensively in the licensing of nuclear projects (U.S. Department of Energy, 1980). It provides predictions of dose based on idealized discharges of radionuclides from the repository system to the biosphere. The individual models used to determine the dose conversion factors are each based on empirical data. The factors are then related to the phenomenology for biosphere transport and uptake by plants, animals, and human beings.

Thus, the code is closely tied to existing data and is based on methodology that has been considered satisfactory for a number of years. Because of the simplicity of the discharge model of radionuclides, use of the code should provide a conservative upper bound estimate of the dose (INTERA, 1983). However, the code is intrinsically not susceptible to validation. Examples are not available in nature with which doses predicted with the code can be compared. In other words, it is not feasible to compare a predicted dose to the "real" dose. It is in this sense that dose assessment models cannot, strictly speaking, be validated.

ONWI's Preliminary Performance Assessment Plan (1983) states on page 133 that codes reflecting ICRP-30 methodology will be used. However, PABLM is based on an ICRP-2 model (ICRP, 1959). This use of ICRP-2 methodology is defended in Sec. 2.4 (Advantages and Limitations of the Approach) of ONWI-446. Because PABLM is well documented and well understood, and represents a rather large investment, arguments can be made to use this code until ICRP-30 codes are developed to a comparable level of trust; however, the transition to reliance on an ICRP-30-based code should be addressed.

3.15.8 Proposed ONWI Application

As a site assessment code for biosphere radionuclide transport and radiation dose, PABLM can be used as a human dose model for ingestion and external exposure through different pathways, both for environmental radiological exposures under normal operations and for environmental radiological exposure after accidents. The code could be used to assess the performance of a geologic radioactive waste repository system both during operation and after postclosure releases. Because the dosimetry model is independent of the origin of the radionuclides, PABLM and related codes are applicable to a nuclear waste repository in salt.

3.15.9 Relationship of Model to Other Codes

Many models and codes for biosphere transport and for radiological dose to humans are available; relevant tabulations are found in Science Applications (1981). ARRRG,FOOD performs related calculations restricted to a one-year dose and a committed dose from one year of exposure. Other programs that compute organ dose factors include AERIN, which calculates organ and tissue burdens resulting from acute exposure to a radioactive aerosol; DACRIN, which calculates organ dose from acute or chronic radionuclide inhalation; and SUBDOSA, which calculates external dose from atmospheric release of radionuclides.

PABLM requires the following data libraries: master radionuclide and radiological decay data library RDMLIB, organ data library ORGLIB, aquatic bioaccumulation factor library BIOAC, external radiation dose factor library GRDFLIB, and food transfer coefficient library FTRANSLIB.

The PABLM code can be coupled with the DACRIN code, which models radiation dose from inhaled materials. It can also be used in conjunction with solute transport codes like SWENT, LAYFLO, MMT, GETOUT, and DPCT (Science Applications, 1981; Thomas et al., 1982). PABLM is incorporated as part of the SCEPTER (Brecher and Pearson, 1983) technology package. The version of PABLM used in SCEPTER does not evaluate inhalation dose; this calculation can be performed by the code DACRIN, which is also in the SCEPTER package. These two codes can be used to evaluate the total dose commitment associated with predicted radionuclide release rates. PABLM can also be used in conjunction with site subsystem groundwater flow and radionuclide transport codes to assess site subsystem performance. This same approach can be applied to the other subsystems (waste package and repository), although care must be taken in specifying the pathway from the subsystem to the biosphere and the model for discharge to the biosphere itself.

3.15.10 Application of Code to Other Problems

PABLM has been used extensively in the licensing of nuclear projects. The original version of the PABLM code was written to calculate internal and external radiation doses from radionuclides released to the biosphere from a nuclear facility (Napier et al., 1980).

3.15.11 Suitability of Model for Salt Repository Application

Because the dosimetry model is independent of the origin of the radionuclides, PABLM is suitable for salt repository applications. However, there are some limitations in the use of this code for such applications. PABLM is designed to evaluate the dose that occurs within one generation; for example, during the lifetime of an individual. There may be situations where multigenerational effects may be important for long-term releases (Smith et al., 1982; INTERA, 1983). For example, although the present version of PABLM considers the accumulation of radionuclides in farmland as a result of continued irrigation with contaminated water, this accumulation is not considered for more than the time of exposure. Another limitation is in the dose models themselves. The models in PABLM are all based on the formulation of the models in ICRP-2 (ICRP, 1959). More recent developments suggest that some of these models may need to be reviewed (ICRP, 1979).

PABLM can be used in conjunction with site subsystem groundwater flow and radionuclide transport codes to assess site subsystem performance. This same approach can be applied to the other subsystems (waste package and repository), although care must be taken in specifying the pathway from the subsystem to the biosphere and the model for discharge to the biosphere itself.

3.15.12 Peer Review

No peer review of PABLM has been documented.

3.15.13 References for Section 3.15

Brecher, A., and F.J. Pearson, Jr., *The SCEPTER Waste Package Subsystem Computer Model for Performance Assessment*, in Scientific Basis for Nuclear Waste Management VI, D.G. Brookins, ed., Elsevier Science Publishing Co., New York, N.Y. (1983).

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Office of Nuclear Waste Isolation, *Preliminary Performance Assessment Plan for a Nuclear Waste Repository in Salt*, Battelle Memorial Institute, Columbus, Ohio, unpublished manuscript (April 1983).

Science Applications, Inc., *Tabulation of Waste Isolation Computer Models*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-78 (Aug. 1981).

Shriner, C.R., and L.J. Peck, *Inventory of Data Bases, Graphics Packages, and Models in Department of Energy Laboratories*, Oak Ridge National Laboratory Report ORNL/EIS-144 (Nov. 1978).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

Smith, C.B., et al., *Population Risks from Disposal of High-Level Radioactive Wastes in Geologic Repositories*, U.S. Environmental Protection Agency Draft Report EPA-520/3-80-006, National Technical Information Service Pub. No. PB-83-169953 (Dec. 1982).

Thomas, S.D., et al., *A Summary of Repository Siting Models*, U.S. Nuclear Regulatory Commission Report NUREG/CR-2782 (July 1982).

U.S. Department of Energy, *Final Environmental Impact Statement — Management of Commercially Generated Radioactive Waste*, DOE/EIS-0046F (Oct. 1980).

3.16 PHREEQE: A GEOCHEMICAL SPECIATION AND MASS-TRANSFER CODE SUITABLE FOR REPOSITORY PERFORMANCE ASSESSMENT

3.16.1 Code Description

PHREEQE (INTERA, 1983, ONWI-435) is a general geochemistry computational algorithm that can be used by experienced geochemical modelers to compute various properties of a solution under conditions of thermodynamic equilibrium. Properties that can be computed include pH, redox potential, cation and anion concentrations, and distribution of constituents among the various phases in equilibrium at a given temperature, pressure, and solution composition. Chemical kinetics are not treated.

The code tracks the progress of a set of reactions as some external change to the solution occurs, that is, as its temperature is changed or as some chemical compound is added. This tracking must be conducted in a manual or semiautomatic way, that is, a sequence of code runs computes the solution conditions for the corresponding sequence of equilibrium conditions. The user must keep track of the amounts of material that change phase as each phase boundary is crossed, because this is not automatically done by the code. Temperature cannot be computed as a consequence of a series of reactions. It is strictly an external constant supplied by the user.

An important aspect of using this code, which is similar to the EQ3/EQ6 code, is developing adequate input data sets. The most important of these is the thermodynamic data set, which contains equilibrium constants and dissociation constants for all reactions and ion (cation-anion) pairs specified by the user. Two such data sets are available -- one comes with PHREEQE and the other comes with EQ3/EQ6. Experience to date shows that for certain problems, differences between these two thermodynamic data sets can have a major impact on PHREEQE calculations, especially in reaction-path simulations.

Another important input requirement is choosing the equation to calculate the activity coefficient for each constituent ion pair. Although the code provides four choices, it is not clear how applicable any of the available choices is to a salt repository, where solutions would contain high brine concentrations. At least one of the choices is based on the Debye-Hückel theory, which is strictly valid only for very dilute electrolyte solutions having total dimensionless ionic strengths of 0.1 or less.

The model consists of a system of simultaneous, nonlinear, algebraic equations that are solved iteratively by a combination of the continued-fraction and Newton-Raphson methods. An early version of the code was written for an IBM machine, whereas the more recent version described in ONWI-435 was written for a CDC machine. The latter version was written in FORTRAN IV but makes use of some installation-specific features. A summary of PHREEQE was published by NRC (Thomas et al., 1982).

3.16.2 Development Stage

The code as described in ONWI-435 contains several minor revisions as compared with the original version written by the U.S. Geological Survey (Parkhurst et al., 1980) to deal with surface-water and groundwater hydrogeochemical studies. The code package contains a thermodynamic data set and a preprocessor that converts an EQ3/EQ6-compatible thermodynamic data set into one that can be read directly by PHREEQE. However, PHREEQE does not need a preprocessor if the input data are prepared as instructed in its user's manual. Another minor revision is incorporation of the "BDOT" form of the extended Debye-Hückel activity coefficient formula.

3.16.3 Documentation

ONWI-435 was prepared in accordance with NUREG-0856 (Silling, 1983) and is quite complete. Much of the theory section and parts of the user's manual have been taken verbatim from previously published material. The user's manual section and, in

particular, the two example problems illustrate how the code is used. In fact, it is not until these example problems are studied that one gains some appreciation for how the code simulates reaction paths and what its general limitations are. One major weakness of the documentation is its failure to address the range of dilution over which the code is applicable.

A substantial effort is made in ONWI-435 to compare PHREEQE with another geochemistry code, EQ3/EQ6. These comparisons are very useful in illuminating the features and limitations of PHREEQE. While EQ3/EQ6 has more powerful simulation capabilities and is easier to use, PHREEQE is simpler and runs faster.

3.16.4 Performance Specification Review

The internal review of the PHREEQE model conducted by INTERA is presumably the basis for Sec. 2 of ONWI-435. According to this section, PHREEQE meets the following requirements:

1. Incorporation of a general algorithm with aqueous species and solid-phase identities set by user input.
2. Ability to handle temperature variation.
3. Ready availability of source code and adequacy of documentation.

The PHREEQE code also met the requirement for a rather rapidly executing mass-transfer code for assessing performance over long periods in the far field, for evaluating test data, and for calculating the need for data acquisition.

The model is of the ion-association type, in which a set of mass-action equations are specified for each ion pair and a set of mass-balance equations for each element considered. These equations are coupled by activity coefficients for each aqueous species and solved numerically. Four ways to express activity coefficients are provided.

No external review is documented in ONWI-435.

3.16.5 Code Design Review

The internal review of the PHREEQE code conducted by INTERA was presumably the basis for portions of Sec. 3 of ONWI-435. This section specifies the methods used to solve the governing equations.

The code solves a set of nonlinear algebraic equations using a combination of a continued-fraction approach and a Newton-Raphson approach. The independent unknowns are the electron and hydrogen ion activities, the activities of the user-specified "master species," and the amounts of mineral mass transferred to the aqueous phase. Activity coefficients are calculated using either the Debye-Hückel or Davies'-based formulas.

No external review is documented in ONWI-435.

3.16.6 Verification

ONWI 435 describes one test of PHREEQE in which comparisons were made with hand-calculated results. It also describes several code-to-code tests on benchmark-type problems. The sensitivity of the code to changing from one thermodynamic data set to another was also examined, as was the influence of alternative ways to input carbon species data. No verification tests have been reported for salt brine conditions.

1. Speciate Major Ions of Seawater. The purpose of the first problem was to verify coding in PHREEQE by comparing model results with those from hand calculations. Four cations, five anions, and the thermodynamic data set that comes with the code were used. The percentages of total ion concentrations represented by ion pairs and free ions were compared, and agreement was quite good.
2. Speciate Full Seawater Analysis. The purpose of the second problem was to compare PHREEQE results with those calculated using the original PHREEQE, WATEQF/WATEQ2 (Plummer et al., 1976), and EQ3 codes. Also examined was the effect of using two different thermodynamic data sets and of using the total alkalinity versus the total carbonate method of entering carbon species data. As far as the carbon input via total alkalinity versus total carbonate, the differences in carbon species concentrations are on the order of 5% or less. When two independent thermodynamic data sets are used as input to PHREEQE, the differences in species concentrations are generally on the order of 5%. If two different expressions for computing activity coefficients are used (comparison of new and old versions of PHREEQE), the differences in species concentrations are generally 1% or less. When PHREEQE is compared with EQ3 and with WATEQF/WATEQ2, the differences are generally small but larger for selected species concentrations. Calculations of saturation indices for selected minerals were generally much more sensitive to code and to thermodynamic data set than to species concentration. The greatest differences generally occurred when the two different thermodynamic data sets were used with the same model.
3. Dissolve Microcline in Dilute Hydrochloric Acid. The purpose of the third problem was to illustrate and compare the reaction-path-modeling and phase-boundary-locating capabilities of PHREEQE with EQ3/EQ6 and hand calculations. Calculated equilibrium phase boundaries agreed with those obtained by hand calculations for a given thermodynamic data set, but there were large differences for the two different data sets.

PHREEQE requires greater user input than the EQ6 code to perform reaction-path simulations. First, several separate runs of PHREEQE are required, all of which require carefully selected input specifications. Second, the user must keep track of mineral assemblages as the phase boundaries are crossed. EQ6 simulates the entire reaction path automatically. This aspect of PHREEQE suggests that the code be used only by experienced geochemistry modelers.

Results showed that both PHREEQE and EQ6 are capable of producing essentially the same set of results when used with the same data sets. Results also showed that if two different data sets are used with the same code, the results can be quite different.

3.16.7 Validation

No validation has been reported. On page 56 of ONWI-435, the authors argue that the code can be said to have been validated because the model is based on sound thermodynamic principles that have never been proven wrong. Such arguments do not constitute validation. It is true that most of the equations upon which the code depends are statements of sound physical principles like thermodynamic equilibrium. But, because of the limits of validity of equations such as those used to compute activity coefficients and because not all real systems can be completely specified by a few equations (even if these equations are based on physical principles), it cannot be said, *a priori*, that this code gives a valid representation of reality. It must, in fact, be demonstrated that for certain systems obeying well-defined limitations, the code gives reliable predictions.

ONWI 435 further states (p. 56) that if discrepancies between PHREEQE results and observations are found, the error could most likely be traced to the uncertainty in the data used to describe equilibrium constants or the inapplicability of the activity coefficient correlations to the problem at hand. In other words, the wish is to place the burden of the validity of the model entirely on the validity of the input data. Even if this approach were appropriate, it would have to be demonstrated.

3.16.8 Proposed ONWI Application

ONWI proposes to use PHREEQE for geochemistry calculations in the far field where equilibrium conditions are likely to obtain. In the near-field environment, where equilibrium is less likely to be attained, this code will be used for bounding calculations.

3.16.9 Relationship of Model to Other Codes

The PHREEQE code can be operated as a stand-alone computational algorithm. It does not require a preprocessor for its input data unless data sets not originally designed for this code need to be transformed. This code will probably be used in

conjunction with hydrological transport codes like SWENT, because it can be used to predict the phase equilibrium (i.e., mass fraction in solution versus that in solid phase) of various chemical compounds including those containing radionuclides. As the fluid carrying dissolved radionuclides passes through different media, new calculations using PHREEQE can be performed to estimate any changes in solubility.

3.16.10 Application of Code to Other Problems

Potential applications of the code include predicting the equilibrium distribution of various radioactive compounds between the dissolved and solid states for a wide range of user-specified solution compositions and thermodynamic variables. Hence, the code can be used in conjunction with fluid transport codes to determine the mass of various radionuclides that are carried away in solution under well-defined, constant, equilibrium conditions. Several example problems are discussed in Parkhurst et al. (1980).

3.16.11 Suitability of Model for Salt Repository Application

A fundamental limitation of PHREEQE is its applicability to very dilute electrolyte solutions. It is not evident from ONWI documents that PHREEQE's applicability to concentrated brine solutions has been addressed.

3.16.12 Peer Review

There is no documented evidence of peer review.

3.16.13 References for Section 3.16

INTERA Environmental Consultants, Inc., *A Geochemical Speciation and Mass Transfer Code Suitable for Nuclear Waste Performance Assessment*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-435 (April 1983).

Parkhurst, D.L., et al., *PHREEQE: A Computer Program for Calculations*, U.S. Geological Survey Water Resources Investigations Report 80-96 (1980).

Plummer, L.N., et al., *WATEQF: A Fortran IV Version of WATEQ, A Computer Program for Calculating Chemical Equilibrium of Natural Waters*, U.S. Geological Survey Water Resources Investigations Report 76-13 (1976).

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Thomas, S.D., et al., *A Summary of Repository Siting Models*, prepared by GeoTrans, Inc., for U.S. Nuclear Regulatory Commission, NUREG/CR-2782 (July 1982).

3.17 SALT4: A TWO-DIMENSIONAL DISPLACEMENT DISCONTINUITY CODE FOR THERMOMECHANICAL ANALYSIS IN BEDDED SALT DEPOSITS

3.17.1 Code Description

SALT4 (INTERA, 1983, ONWI-429) is a two-dimensional thermomechanical code for predicting temperatures, deformations, and stresses in a repository located in bedded salt. In the SALT4 model, all space is divided by a horizontal plane (the earth's surface) into two infinite half-spaces, with the earth's surface taken to be isothermal. In the lower half-space, between two horizontal planes, are the excavated rooms (taken to be infinitely long), which alternate with support pillars. The lower of the two below-surface horizontal planes is at floor level, with the upper one at ceiling level. Buried under the centerline of each room and running parallel to its length is a row of nuclear waste packages represented by a line source of heat. The volume between the two below-surface planes is referred to as the seam.

The lower half-space is taken to have constant, isotropic thermal conductivity, and the heat flow equation is solved analytically for a line source of heat. The heat source can be a general function of time. The rock above and below the seam is taken to be a homogeneous, transversely isotropic elastic medium. The salt pillars within the seam are modeled as exhibiting linear elastic or creep (elastoviscous) behavior.

For the nonseam rock mass and for the line heat source, the thermomechanical equations are solved analytically for stress and displacement. The analytic line-source temperature solution plus geostatic stresses are used to determine the elastic or creep response of the salt pillars. The displacement-discontinuity method is coupled to the line-source solutions to find the total solutions for stress and displacement.

Input to SALT4 consists of system geometry, rock properties (thermal properties, density, elastic moduli, and creep parameters), initial conditions, and time behavior of heat sources. Output includes temperatures, stresses, and displacements.

SALT4 incorporates (1) alternative excavation sequences, (2) viscoelastic behavior in the pillars adjacent to the rooms, (3) transversely isotropic elastic moduli, and (4) a creep law consistent with laboratory experimental data for salt. It offers computational efficiency and requires few input data.

Limitations of the code include: (1) the model is limited to two dimensions; (2) only heat conduction is considered; (3) variations in the thermal properties of the rock mass (including thermal conductivity) with temperature are neglected; (4) nonlinear deformation is not considered for the general rock mass; and (5) creep is allowed only in the pillars.

SALT4 is written in FORTRAN IV for use on a CDC CYBER 176 computer.

3.17.2 Development Stage

SALT4 is ready for use.

3.17.3 Documentation

SALT4 is documented in ONWI-429 in accordance with the NUREG-0856 (Silling, 1983) format. While generally well written, ONWI-429 is less than clear in describing the mathematical model on which SALT4 is based. For instance, relatively unfamiliar notation is used in the first equation (Eq. 2.1). Further, what elastic properties do the pillars have when they are taken to be elastic? Also, the authors should clarify why the inhomogeneity introduced by the rooms is apparently ignored in the calculation of temperature. Finally, "displacement-discontinuity" is not well defined, and the discussion of the displacement-discontinuity method is unclear.

3.17.4 Performance Specification Review

No external performance specification review has been documented.

3.17.5 Code Design Review

No code design review has been documented.

3.17.6 Verification

Two verification tests are described in ONWI-429. In the first of these, the agreement between the SALT4 result and that from an independent code (SNEAKY) is excellent, except near the zero-tension level. The small but systematic discrepancies near the zero-tension level should be explained. Agreement was excellent in the second test, which involved comparing SALT4 output with an analytical solution. Table 4-1 doesn't seem to be a comparison and needs further discussion.

3.17.7 Validation

SALT4 was used to simulate the heater tests performed in Project Salt Vault (Starfield and McClain, 1973). Except for an approximately 10% discrepancy beyond 800 days in the plot for gauge-159, there was good agreement between SALT4 predictions and observed experimental behavior. However, the above discrepancy should be explained.

3.17.8 Proposed ONWI Application

SALT4 is suitable for repository assessment. In particular, it can evaluate alternative patterns and sequences of excavation or waste package emplacements.

3.17.9 Relationship of Model to Other Codes

As an analytically based code, SALT4 can be used to verify other fully numerical codes like DOT and VISCOT. SALT4 does not need input from, nor does it provide output to, other codes.

3.17.10 Application of Code to Other Problems

No application is known other than Project Salt Vault (Starfield and McClain, 1973). This application was used to validate the model.

3.17.11 Suitability of Model for Salt Repository Application

Although salt deforms plastically, only the pillars are so treated in SALT4. Also, horizontal wall deformation and the inhomogeneity of the rooms are ignored.

3.17.12 Peer Review

Peer review has not been completed.

3.17.13 References for Section 3.17

INTERA Environmental Consultants, Inc., *SALT4: A Two-Dimensional Displacement Discontinuity Code for Thermomechanical Analysis in Bedded Salt Deposits*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-429 (1983).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

Starfield, A.M., and W.C. McClain, *Project Salt Vault: A Case Study in Rock Mechanics*, International Journal of Rock Mechanics and Mining Sciences and Geomechanics Abstracts, 10:641-657 (1973).

3.18 SPECTROM-58: A SENSITIVITY STUDY OF BRINE TRANSPORT INTO A BOREHOLE CONTAINING A COMMERCIAL HIGH-LEVEL WASTE CANISTER

3.18.1 Code Description

SPECTROM-58 (Ratigan, 1983a, ONWI-384) is a two-dimensional (Cartesian) finite-element code for predicting brine transport in natural rock salt as a function of

time. The model on which the code is based views the rock salt as consisting of individual crystals, with some of the pore space between the crystals being hydraulically connected and the rest unconnected.

A rock salt crystal typically contains small inclusions of liquid brine. In the presence of a temperature gradient, these inclusions migrate up the gradient to the hotter region. (Dissolution of salt at the hot end of the inclusion and its going out of solution at the cool end have been invoked to account for this migration.) Such thermally driven transport of brine within salt crystals is one of two brine transport mechanisms in the SPECTROM-58 model. The other is the pressure-driven transport of brine through connected pore space. When migrating brine inclusions reach the boundary surface of an individual crystal, the model assumes that they pass through that surface into the pore space and never reenter the same, or any other, crystal.

Brine that enters connected pore space in this manner contributes to the brine flow through that space. In the conceptual SPECTROM-58 model (i.e., the model on which the SPECTROM-58 code is based), the very discontinuous salt crystal matrix is replaced by a continuous volume of salt, and an equation expressing conservation of inclusions in that continuous volume is formulated. This equation contains a term that represents the loss of inclusions at crystal boundaries. The derivation of this equation assumes that all brine inclusions are of uniform size and shape and remain so.

A second equation is derived by (1) considering the connected pore space to be fully saturated with brine, (2) assuming the connected-pore-space brine flows according to Darcy's equation, (3) assuming that flow is driven by pressure gradients only, and (4) writing down a mass conservation equation for the connected-pore-space brine. This conservation equation contains a source term that takes into account the flux of inclusion-brine into the connected pore space. Permeability can be anisotropic, and the salt matrix and the brine are both taken to be compressible. A third model equation is the empirical equation that expresses the inclusion velocity within crystalline salt as a function of the temperature and temperature gradient.

The three model equations constitute the basis for the SPECTROM-58 code. Input to the code consists of system geometry, temperature field, properties of the brine and salt, and initial and boundary conditions. Output includes pressures, values of inclusion density, and the components of the two-dimensional inclusion velocities. The Galerkin finite-element method is used to obtain output from input.

Limitations of SPECTROM-58 include those arising from the above-noted assumptions. Other, and probably very significant, limitations are that the SPECTROM-58 model does not take into account absorption of water molecules by the salt crystals or dissolution of salt into the connected-pore-space brine. Even if the brine has an equilibrium concentration of salt at one temperature, it will no longer be in equilibrium when it convects to a warmer (or cooler) location.

The SPECTROM-58 code is presumably written in FORTRAN. However, the code documentation specifies neither the language nor the type of computer on which the code has been run.

3.18.2 Development Stage

SPECTROM-58 is complete and operational.

3.18.3 Documentation

SPECTROM-58 is documented in ONWI-384 and in a second document by Ratigan (1983b). These documents do not and were never intended to follow the NUREG-0856 (Silling, 1983) format. Nevertheless, they contain many of the elements required by that format, including a reasonably complete derivation of the mathematical model, a thorough description of the finite-element solution to the model equations, a report of a verification test, and parts of a user's manual.

The following points pertain to the derivation of the mathematical model as presented in ONWI-384.

1. The assumption that all brine inclusions have the same size and shape is probably weak. Rather than making this assumption, it may be possible to base the theory on average properties (volume and velocity) of the inclusions.
2. The mechanism that makes the inclusions migrate to a region of higher temperature should also make the connected-pore-space brine move in the same direction. But, the SPECTROM-58 model excludes all transport except that caused by pressure gradients.
3. Equation 2-3 in ONWI-384 is

$$Q = \frac{|\tilde{V}|}{D} \rho$$

where:

Q = flux of brine inclusion density across a crystal surface per unit volume of crystal,

$|\tilde{V}|$ = magnitude of inclusion velocity \tilde{V} ,

D = ratio of crystal volume to crystal surface area, and

ρ = brine inclusion density.

As it appears, Eq. 2-3 is incorrect. The correct equation, found by averaging over the entire crystal, is

$$Q = \frac{|\tilde{V}|}{D} \overline{\rho \tilde{n} \cdot \frac{\tilde{V}}{|\tilde{V}|}},$$

where $\overline{\rho \tilde{n} \cdot \frac{\tilde{v}}{|\tilde{v}|}}$ denotes the average value $\rho \tilde{n} \cdot \frac{\tilde{v}}{|\tilde{v}|}$ (\tilde{n} = outward normal to the crystal surface) over the crystal surface.

This average value will always be nonnegative and could be zero. For example, it would be zero for a crystal that is infinitely long and whose axis is in the direction of the temperature gradient.

4. The assumption in the model that the connected pore space is fully saturated seems highly unlikely to be realized in a salt formation selected for its dryness.

3.18.4 Performance Specification Review

No performance specification review is known to have taken place.

3.18.5 Code Design Review

No code design review is known to have taken place.

3.18.6 Verification

One verification test, for a very simple geometry, has been made. As the number of mesh elements increased and the size of the time steps decreased, the finite-element solution more closely approximated the analytic solution. The number of elements was increased to eight and no higher; for this number, the discrepancy between the SPECTROM-58 solution and the analytic solution was good for the pressure curves (for which the analytic solution was continuous) but not so good for the inclusion density curves (for which the analytic solution was discontinuous).

3.18.7 Validation

SPECTROM-58 has not been validated.

3.18.8 Proposed ONWI Application

SPECTROM-58 would be used for repository assessment. In fact, it has already been used to estimate the rate at which inclusion brine is transported to the waste package (Ratigan, 1983a). SPECTROM-58 might also be used to study the flow of water through the salt formation in which the repository is embedded.

3.18.9 Relationship of Model to Other Codes

SPECTROM-58 requires input temperatures from a thermal transport code like HEATING6, DOT, TEMP, or SALT4. The code MIGRAIN (Rickertsen, 1980), like SPECTROM-58, simulates the migration of brine inclusions but, unlike SPECTROM-58, it has no capability for simulating the flow of brine through the connected pore space of a salt formation.

3.18.10 Application of Code to Other Problems

No other application for SPECTROM-58 is currently envisaged.

3.18.11 Suitability of Model for Salt Repository Application

SPECTROM-58 simulates the transport of brine in natural rock salt in the presence of temperature and pressure gradients. However, the code's neglect of water absorption by the salt and of dissolution of salt into the brine may cause significant inaccuracies.

3.18.12 Peer Review

SPECTROM-58 has not been peer reviewed.

3.18.13 References for Section 3.18

Ratigan, J.L., *A Sensitivity Study of Brine Transport into a Borehole Containing a Commercial High-Level Waste Canister*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, Topical Report RSI-0185, ONWI-384 (1983a).

Ratigan, J.L., *Input Guide for SPECTROM-58*, Technical Letter Memorandum RSI-0090, RE/SPEC, Inc., Rapid City, S.D. (1983b).

Rickertsen, L.R., *Brine Migration in a Bedded Salt Nuclear Waste Repository*, Proc. Heat Transfer in Nuclear Waste Disposal, Annual Winter Meeting of American Society of Mechanical Engineers, HTD, Vol. II, p. 101 (Nov. 16-21, 1980).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

3.19 STAFAN: A TWO-DIMENSIONAL CODE FOR FLUID FLOW AND THE INTERACTION OF FLUID PRESSURE AND STRESS IN FRACTURED ROCK

3.19.1 Code Description

STAFAN (stress and flow analysis) is a two-dimensional (Cartesian or axisymmetric) finite-element code (INTERA, 1983, ONWI 427) developed to treat either rock deformation or groundwater flow, or both of these processes coupled together. Transient flow through both unfractured and fractured systems can be simulated. In the case of flow through a fractured system, STAFAN uses a dual-porosity approach, a discrete-fracture approach, or a combination of the two. The dual-porosity approach assumes that the system has an extensive network of connected fractures and then conceptually divides the porous and fractured medium into two everywhere-coexisting continua. Flow then takes place within each continuum, with fluid being exchanged between the two continua according to a specified rule. The discrete-fracture approach assumes the system being simulated contains just a few fractures, with the geometry of each fracture being described in detail. In both approaches, input to STAFAN consists of system geometry; properties of the fluid, porous matrix, and fractures; and initial and boundary conditions.

The primary output in the dual-porosity case is hydraulic head at the nodal points of a finite-element network as a function of time. In the discrete fracture case, the primary output consists of rock displacements and fluid pressures at nodal points, as a function of time. In both cases, output is obtained from input by using the Galerkin finite-element method to solve appropriate equations for fluid flow in a deformable medium. Permeability can be anisotropic and heterogeneous.

Limitations of the STAFAN code are: (1) it cannot simulate processes in which the role of temperature is dominant, (2) it cannot simulate inelastic deformations of a rock mass, (3) the elastic stress-strain relationship is linear, (4) deformations are taken to be small, (5) the porous medium is mechanically isotropic, (6) flow is assumed to be fully saturated, (7) the porous medium does not absorb water or go into solution, and (8) it is restricted to using two-dimensional Cartesian coordinates or axially symmetric cylindrical coordinates. STAFAN is written in FORTRAN IV for use on a CDC Cyber 176 computer.

3.19.2 Development Stage

STAFAN is ready for use.

3.19.3 Documentation

STAFAN is documented in ONWI-427 in the NUREG-0856 (Silling, 1983) format. The documentation is reasonably good, with the mathematical formalism appearing to be particularly well handled. However, ONWI-427 does far too little to develop in its

readers an intuitive physical understanding of the processes being modeled. Indeed, relatively simple, basic physical processes are disguised in abstract mathematics. While the abstract mathematics is necessary, the basic physical processes should be presented more explicitly.

For example, what is meant by "coupled groundwater flow and rock deformation" (p. 1)?* The simulation of these coupled phenomena is, after all, STAFAN's main thrust. Presumably, ONWI-427's authors had in mind here two means by which such coupling could occur. First, an increase in groundwater pressure could cause the rock matrix to expand vertically upward as the water pressure carries more of the geostatic load. Second, rock deformations that reduce porosity will increase pressure. Since these couplings are so basic to ONWI-427, they should be described and illustrated in figures. The physics of the coupling should be reviewed and examples presented with typical numbers.

Also, because Eq. 2.35 (p. 16) is presented in general tensor notation, the physics behind the equation is obscured. It would be much easier to understand the origin of the rightmost term (the one due to displacement of the solid boundaries) if a figure were presented along with the derivation of the equation. The figure should show the fracture lying along one of the two axes and should indicate the displacements of the solid boundaries. The equation could be readily derived from the figure and then the axes could be rotated to obtain the general tensor form shown on page 16.

Other comments about the documentation in ONWI-427 are as follows.

1. The dual-porosity flow equations are presented in Sec. 2.2.4. Where is the deformation equation? Is it Eq. 2.1?
2. Equation 2.3 is referred to as one of the governing equations for deformation in the fracture (p. 7). What does "deformation in the fracture" mean? Deformation of the fracture should be governed by a nonlocal, not a local, equation.
3. On page 10, simultaneous changes in porosity and density of the solid are considered. An equation appears to be missing -- one that relates these changes to each other, to the fluid pressure, and to the stress.
4. At the top of page 12, three assumptions are made. Why is the first assumption ($v_{is} \frac{\partial p}{\partial x_i} \ll \frac{\partial p}{\partial t}$) justified? The third assumption implies that the fluid is either slightly compressible or incompressible, rather than just incompressible. The second assumption, that the solid grains are incompressible, is not justified when the fluid (namely, water) is slightly compressible, because rock and water compressibilities are of the same order of magnitude, both being roughly $5 \times 10^{-6} \text{ psi}^{-1}$.

*Page numbers in Sec. 3.19 are from ONWI-427.

3.19.4 Performance Specification Review

Internal performance specification reviews by INTERA and ONWI have been completed.

3.19.5 Code Design Review

Internal code design reviews by INTERA and ONWI have been completed.

3.19.6 Verification

The STAFAN code was tested by comparing its solutions to three problems to published analytic solutions to the same problems. The problems were selected to represent different types of physical situations.

The first problem was to determine well drawdown as a function of time for the case of water flow to a pumped well that penetrates all the way through a confined aquifer. A single vertical fracture intersects the well at the center of a square region. Thus, this first problem provides a test of STAFAN's capability for simulating discrete fractures. For this problem, agreement between the STAFAN solution and the analytic solution was excellent.

The second problem provided a test of STAFAN's capability for simulating formations containing many distributed fractures of unknown geometry, that is, a test of STAFAN's dual-porosity formalism. This problem was to calculate well drawdown versus time in the case of a well penetrating a confined, water-bearing formation, which was fractured as described. Excellent agreement was obtained between the STAFAN and analytic solutions in this case as well.

The third problem, unlike the first two, involved coupled flow and deformation. Also, the flow in the third problem was through a porous medium, not a fractured one. This problem consisted of determining the two-dimensional plane elastic deformation of a fully saturated porous medium subject to a specified pressure loading over a horizontal strip on the top surface of the medium. ONWI-427 makes the puzzling assertion that there is no flow other than at the top surface. But, if so, how does the water get to the top surface? Because the description of this problem is less than clear, it would be nearly impossible to duplicate the test, given that description alone. Near the top surface (zero depth), agreement between STAFAN and the analytic solution is excellent in the case of excess pore pressure along a horizontal line and good (within ~5%) in the case of excess pore pressure along two vertical lines. Near the bottom surface of the porous medium, the STAFAN and analytic results are not in agreement, but agreement is not expected because the analytic solution assumes infinite depth, whereas STAFAN assumes a depth of 80 meters.

Although the impressive agreement between STAFAN and analytic solutions in the three problems constitutes significant verification, further verification tests are needed. For example, STAFAN's capability to simulate coupled fluid flow and

deformation when the porous medium is fractured has not been tested. Also, STAFAN should be tested against other codes for problems having more complex geometry than the three verification problems detailed in ONWI-427.

3.19.7 Validation

STAFAN has not been validated.

3.19.8 Proposed ONWI Application

STAFAN will be used in repository and site assessment.

3.19.9 Relationship of Model to Other Codes

An analysis of water flow by STAFAN can serve as input to the solute transport codes FTRANS and SWENT. Also, STAFAN can be used to check assumptions about the effect of deformation on pressure and velocity distributions made by the flow codes NETFLO and SWENT.

3.19.10 Application of Code to Other Problems

No other applications of STAFAN are known.

3.19.11 Suitability of Model for Salt Repository Application

STAFAN should not be applied to the flow of water through salt because: (1) salt is plastic, whereas STAFAN assumes the rock is elastic (or bilinear inelastic at the joints), and (2) STAFAN does not take into account that water is absorbed by salt and that salt dissolves into the flowing water.

3.19.12 Peer Review

STAFAN has not been peer reviewed.

3.19.13 References for Section 3.19

INTERA Environmental Consultants, Inc., *STAFAN: A Two-Dimensional Code for Fluid Flow and the Interaction of Fluid Pressure and Stress in Fractured Rock for Repository Performance Assessment*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-427 (April 1983).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

3.20 STEALTH-2D HYDROLOGICAL MODEL: A LAGRANGE EXPLICIT FINITE-DIFFERENCE CODE FOR SOLID, STRUCTURAL, AND THERMOHYDRAULIC ANALYSIS

3.20.1 Code Description

STEALTH is a package of explicit finite-difference codes developed to solve time-dependent, nonlinear problems in continuum mechanics and time-dependent problems in fluid flow. STEALTH-2D is a two-dimensional planar or axisymmetric thermomechanical code (Hofmann, 1976). The STEALTH-2D HYDROLOGICAL MODEL is a two-dimensional planar or axisymmetric code that solves the equations of fluid flow in a porous medium (Hofmann and Hart, 1979, ONWI-256). When STEALTH-2D predicts thermally induced rock fracturing, the STEALTH-2D HYDROLOGICAL MODEL can be coupled with it to predict water flow through the fractures. (Only the hydrological model was available to Argonne for review.) The codes in the STEALTH package, other than STEALTH-2D HYDROLOGICAL MODEL, are proprietary and therefore unavailable (Casey, 1983). This situation makes the STEALTH-2D HYDROLOGICAL MODEL of limited utility, since explanatory material needed to use STEALTH-2D HYDROLOGICAL MODEL is contained only in the documentation of the proprietary codes.

Input to STEALTH-2D HYDROLOGICAL MODEL consists of the geometry of the flow region; values for liquid viscosity, compressibility, and density; values of the permeability and porosity of the porous medium; boundary conditions; and the initial pressure as a function of position. Output is fluid pressure and flow as a function of position and time. The equations solved by the model are the Darcy equation, the mass conservation equation, and the equations for fluid potential piezometric head and fluid compressibility.

In addition to being restricted to two-dimensional geometries, the STEALTH-2D HYDROLOGICAL MODEL code has the following limitations: (1) dimensions must be such that Darcy flow is legitimate; (2) the spatial region modeled must be homogeneous, although the permeability can be anisotropic; (3) it is assumed that the porous medium does not dissolve into the fluid; and (4) the product of the fluid compressibility and the pressure is assumed to be much less than one. ONWI-256 specifies neither the language in which STEALTH-2D HYDROLOGICAL MODEL is written nor the type of computer on which the code has been run.

3.20.2 Development Stage

STEALTH 2D HYDROLOGICAL MODEL is ready for use within the constraints imposed by the unavailability of STEALTH-2D as mentioned in Sec. 3.20.1.

3.20.3 Documentation

The documentation in ONWI-256 is generally good, but incomplete. Because it was written prior to issuance of NUREG-0856 (Silling, 1983), it does not follow those guidelines. In particular, ONWI-256 uses the term "validation" to mean what NUREG-0856 defines as "verification," and the document does not include a user's manual.

Aside from the NUREG-0856 guidelines, the ONWI-256 documentation is deficient in three respects. First, it is incomplete in that the reader is referred to Ref. 5 of ONWI-256, a proprietary document, for important explanatory material. Second, the types of boundary conditions required for the solution of Eq. 2.10 should be discussed. Third, ONWI-256 assumes that the fluid density is constant while the fluid compressibility is nonzero.

It is possible to have both constant fluid density and nonzero compressibility only if the pressure is constant as a function of position and time. In any problem of practical interest, this condition will not be realized. Actually, it is not necessary to assume both constant density and nonzero compressibility to derive Eq. 2.10 of ONWI-256, the basic equation of the model. One should instead assume nonzero compressibility and compressibility constant with respect to pressure, and that the product (dimensionless) of pressure, p , and compressibility, β is small compared to one. Then Eq. 2.6 can be solved to obtain the following solution:

$$\rho = \rho_0 \exp [\beta p] = \rho_0 [1 + \beta p + \dots]$$

where the subscripts have been dropped. According to this solution, the fluid density ρ is nearly, but not strictly, constant. Using this solution, Eq. 2.10 can be derived by dropping terms of order βp . The derivation of Eq. 2.10 is quite confusing as written because the text states that ρ is constant but the nonzero β requires that it not be constant. In fact, it is not constant, but varies with p as indicated in the above solution.

3.20.4 Performance Specification Review

Performance specification review has not been carried out.

3.20.5 Code Design Review

Code design review has not been carried out.

3.20.6 Verification

Three verification tests were applied to the model: a potential boundary condition test, a fluid-flow boundary condition test, and a pressurized well-bore simulation test, all of which involved comparisons with analytical solutions. All tests assumed isotropic hydraulic conductivity, porosity and hydraulic conductivity that are constant in space, a slightly compressible fluid, and an incompressible porous matrix. In

the second test, a discrepancy between the code solution and the analytic solution occurs at later times. This discrepancy arises because the code solution assumed a compressible fluid while the analytic solution assumed an incompressible fluid. In the first and third tests, there was very close agreement between the code and analytic solutions. Taken together these tests provide significant verification of STEALTH-2D HYDROLOGICAL MODEL code. However, many more verification tests should be made, particularly some involving two dimensions.

3.20.7 Validation

No validation tests were reported in ONWI-256.

3.20.8 Proposed ONWI Application

STEALTH-2D HYDROLOGICAL MODEL will be used in repository assessment. It is suitable for predicting water flow through fractured rock that had low permeability before fracturing. Because of the considerations noted in Sec. 3.20.11, it is not suitable for use in the salt bed itself.

3.20.9 Relationship of Model to Other Codes

The extent of rock fracturing predicted by STEALTH-2D can be converted into input data for STEALTH-2D HYDROLOGICAL MODEL.

3.20.10 Application of Code to Other Problems

In its two-dimensional axisymmetric mode, this model could be useful in modeling the behavior of an aquifer in contact with a gas or oil reservoir.

3.20.11 Suitability of Model for Salt Repository Application

STEALTH-2D HYDROLOGICAL MODEL should not be applied to water seeping through salt. Salt goes into and out of solution readily, and this phenomenon is not taken into account in the model. However, as noted in Sec. 3.20.8, the model is suited for modeling water flow in insoluble fractured rocks lying, say, above a repository.

3.20.12 Peer Review

No formal peer review of STEALTH-2D HYDROLOGICAL MODEL has been carried out.

3.20.13 References for Section 3.20

Casey, L., Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, personal communication (Sept. 1983).

Hofmann, R., *STEALTH: A Lagrange Explicit Finite-Difference Code for Solids, Structural, and Thermohydraulic Analysis, Vol. 1: User's Manual*, prepared by Science Applications, Inc., San Leandro, Calif., for Electric Power Research Institute, Palo Alto, Calif., EPRI NP-260 (1976).

Hofmann, R., and R. Hart, *Hydrological Model in STEALTH 2D Code*, prepared by Science Applications, Inc., San Leandro, Calif., for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-256 (Oct. 1979).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

3.21 SWENT: A THREE-DIMENSIONAL FINITE-DIFFERENCE CODE FOR SIMULATION OF FLUID, ENERGY, AND SOLUTE RADIONUCLIDE TRANSPORT

3.21.1 Code Description

SWENT (INTERA, 1983, ONWI-457) uses a finite-difference technique to simulate steady state and transient three-dimensional transport processes, including fluid flow, heat flow, chemically inert contaminant transport, and radionuclide transport in heterogeneous geologic media. The code is generally applicable to local and regional flow conditions, with or without thermal and salinity effects coupled to the heat and radionuclide transport expressions. Major assumptions include a single liquid phase, laminar (Darcy) flow, first-order salt dissolution reaction, linear equilibrium adsorption, and linearly velocity-dependent hydrodynamic dispersion coefficients.

Along with a wide choice of boundary conditions, the available options permit inclusion of radionuclide sources, heat losses to overburden and underburden, recharge due to rainfall, natural flow in the aquifer, and well conditions at the wellhead or well bottom. A leach submodel can be used to compute source rates based on user inputs, or SWENT will accept source rate input supplied directly by the user. Such rates might be obtainable from codes like WAPPA. Another option useful for repository assessment provides for steady state flow of fluid and transient movement of radionuclides.

Input data include system geometry, formation and fluid properties, well bore parameters, radionuclide chain data, nuclide inventories, and waste properties. Output data include Darcy velocities, pressures, temperatures, and solute and nuclide concentrations at all grid blocks. The code was written in FORTRAN IV for use on a CDC CYBER 176 machine and consists of about 15,000 source statements.

SWENT comprises three nonlinear partial differential equations coupled by fluid density and viscosity. A fourth differential equation for radionuclide transport is independent of the first three, except that it uses the velocity field generated as part of its solution. This latter equation does not influence the solution of the first three equations because the radionuclides are assumed to be present in trace quantities. The main algorithm is based on a linearization of the coupled equations.

The aquifer-model equations include (1) the pressure equations, which are a combination of the continuity equations and Darcy's law in three dimensions; (2) the solute concentration equation, which includes terms for production, injection, and salt dissolution; (3) the energy equation, which provides for heat input from radioactive decay; and (4) the radionuclide transport equation, which includes terms for direct source input, production, and radioactive formation and decay. The radionuclide source term can be entered directly or computed by the leach model that is incorporated into SWENT. The leach model assigns each nuclide to either the "unleached from waste matrix," "leached but undissolved," or "dissolved" states. Phases 1 and 2 are coupled by a constant leach rate, whereas phases 2 and 3 are coupled by their solubilities. The unleached phase equation may be solved internally, or data may be taken from another code, such as ORIGEN2. The dissolved-phase equation ignores dispersive transport.

Major limitations in the model are: (1) the code accommodates only a single liquid phase; (2) fully saturated porous media are assumed; (3) Darcy's-law kinetic energy is ignored in the energy balance; (4) fluid viscosity is assumed to be a function of temperature or, alternatively, of concentration; (5) salt dissolution is dealt with as a first-order reaction; (6) adsorption is treated as a linear equilibrium process; (7) dispersion is assumed to be a linear function of velocity; and (8) dispersion and molecular diffusion are considered to be additive.

The partial differential equations are solved by dividing space into a three-dimensional grid and developing finite-difference approximations of the equations for that grid. The method is semi-implicit in that the dependent variables (pressure, temperature, and concentration) appearing in the space derivatives are expressed at the new time level. Because the equations are nonlinear (fluid properties depend on the dependent variables), the difference approximation is not totally stable. Hence, an iterative procedure is used to solve the equations, and convergence criteria are applied to changes in fluid density between iterations. Two methods are available for solution -- ADGAUSS, a reduced-band-width direct-solution method, and L2SOR, a two-line successive overrelaxation method.

3.21.2 Development Stage

The code is fully operational on a CDC CYBER 76 machine. It has been used by INTERA and others for various applications and has undergone limited verification and validation.

3.21.3 Documentation

SWENT has been fully documented in ONWI-457 in accordance with NUREG-0856 (Silling, 1983).

3.21.4 Performance Specification Review

The findings of INTERA's review are contained in their documentation of SWENT in ONWI-457. Relevant results are discussed in Sec. 3.21.1.

3.21.5 Code Design Review

A review of the code design was conducted by INTERA as part of their documentation of SWENT. ONWI-457 states that "the use of second-order correct finite-difference approximations introduces block-size and time-step restrictions [and that] these restrictions, though considerably less stringent than those of explicit methods, depend upon the magnitude of the dispersivity." It also states that "the comprehensive nature of the code may require more computer time and storage requirements relative to a code written specifically for simple problems." The code provides options for finite-difference approximations, either backward or central differences, both in space and time. Although the code was not designed for "double" or "dual" porosity systems, it can be adapted to such simulations in one or two dimensions. Restart capabilities are provided along with two-dimensional contour mapping.

3.21.6 Verification

According to ONWI-457, there are no published analytical solutions for the complete coupled processes addressed by the code. However, 11 simple, idealized problems were available against which to check portions of the code in an uncoupled fashion. Consequently, fluid flow, heat flow, chemically inert component transport, and radionuclide transport coding were checked separately. These 11 cases are described in detail in Ward et al. (1981) and Intercomp Resource Development and Engineering (1976), with the results summarized in ONWI-457.

Of the 11 cases studied, none involved three-dimensional solutions. Three separate cases addressed one-dimensional convection-dispersive transport with constant velocity of an inert component, heat, and a three-membered radioactivity chain, respectively. There were five separate two-dimensional tests. Of these, two involved well-injection problems (constant pressure or constant rate); one addressed inert-component transport; one addressed radionuclide transport along a single fracture, with molecular diffusion into the rock matrix; and one addressed fluid flow and heat convection in a confined, circular aquifer, with heat loss to the overburden and a uniform vertical temperature profile in the aquifer. All of the reported results of the SWENT calculations appeared to agree reasonably well with the analytical results. The effects of choosing coordinate geometries and boundary conditions were quite small for these cases.

3.21.7 Validation

The following three validation studies cited in ONWI-457 are briefly summarized in a single table in that document.

1. Leachate migration from landfill (Sykes et al., 1981), which "validated" fluid flow and trace component transport.
2. Injection, storage, and recovery of heat from a confined aquifer (Sykes et al., 1982), which "validated" coupled fluid and heat flow.
3. Uranium-front movement in the aquifer (Muller et al., 1981), which "validated" fluid flow and trace component transport.

In the above cases, comparisons between calculated results and field observations were reported as having "validated" certain processes modeled by SWENT. The term "validated" in this sense means good agreement under these particular conditions. Such "validation" does not imply the general validity of those portions of the SWENT model in terms of performance assessment for nuclear waste storage purposes.

3.21.8 Proposed ONWI Application

SWENT may prove useful for the following types of analyses:

1. Waste package thermal boundary analyses.
2. Temperature analyses within waste package components.
3. Repository subsystem thermal environment assessment.
4. Fluid conditions in the repository regime.
5. Groundwater flow and hydrologic budget.
6. Radionuclide transport from repository boundary to biosphere.
7. Evaluation of potential human interference.

With the exception of the second item, these possible applications all derive from SWENT's ability to simulate coupled fluid, heat, solute, and radionuclide transport in a general aquifer system. It is not clear from the documentation whether SWENT could be used for analysis of transport processes occurring within the waste package, other than as an aid in establishing the boundary conditions as in the first application. Virtually all of these applications will require the design of failure scenarios and the coordinated use of codes to provide source terms, geochemical effects, and the effects of flow through fractured media.

3.21.9 Relationship of Model to Other Codes

SWENT is a general-purpose, stand-alone code. For transport of radionuclides, an internal leach submodel can be used to generate a source term or, alternatively, source terms can be obtained from an external code like WAPPA and entered as input. To the extent that solubility of radionuclides is a function of solution speciation, geochemical codes like PHREEQE will be required to determine initial solution properties and phase distributions, and to update them as solution and medium properties as well as the temperature and pressure change. Furthermore, SWENT's simulation capabilities will need to be augmented by codes more specifically designed for flow in unsaturated media (TRIPM) and fractured media (FTRANS). For some purposes, it may be possible to replace SWENT with simpler codes, such as NETFLO and FE3DGW or TRIPM, which handles flow in both saturated and unsaturated porous media. Finally, to determine the radiological exposure to man, the output of SWENT can be used for dose-to-man codes like PABLM.

3.21.10 Application of Code to Other Problems

SWENT has been applied to a number of problem situations, including the following:

1. Nuclear waste isolation in various geologic formations, including basalt deposits, salt domes, and bedded salt formations.
2. Heat storage in aquifers.
3. Injection of industrial wastes into saline aquifers.
4. In situ solution mining.
5. Migration of contaminants in landfills.
6. Disposal of municipal waste.
7. Salt-water intrusion in coastal regions.
8. Brine disposal in underground aquifers.
9. Determination of aquifer transport parameters from well-test data.

3.21.11 Suitability of Model for Salt Repository Application

Although ONWI-457 does not indicate how and how well the special problems of salt repositories can be handled by SWENT, it does list some previous applications of SWENT to problems involving brine solutions and salt repositories. These applications

should be reviewed for further information on the topic of suitability. Because SWENT does have the explicit capability of handling salt dissolution, at least in first-order reactions, it may be suitable for addressing questions related to dissolution of a salt repository host material embedded in a multilayered aquifer system. However, the limitations on brine concentration are not readily apparent in the code documentation. Furthermore, on page 57, ONWI-457 states without further elaboration that SWENT cannot be used in the waste package.

3.21.12 Peer Review

No documented peer review was found.

3.21.13 References for Section 3.21

INTERA Environmental Consultants, Inc., *SWENT: A Three-Dimensional Finite-Difference Code for the Simulation of Fluid, Energy, and Solute Radionuclide Transport*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-457 (April 1983).

Intercomp Resource Development and Engineering, Inc., *A Model for Calculating Effect of Liquid Waste Disposal in Deep Saline Aquifers, Part I: Development, and Part II: Documentation*, National Technical Information Service Pub. No. 26903 (1976).

Muller, A.B., et al., *Geochemical Parameters Used in the Bedded Salt Reference Repository Risk Assessment Methodology*, Sandia National Laboratories Report SAND81-0557 and U.S. Nuclear Regulatory Commission Report NUREG/CR-1997 (1981).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

Sykes, J.F., et al., *Numerical Simulation of Thermal Energy Storage Experiment Conducted by Auburn University, Vol. III: Geosphere Transport Model Validation*, prepared by INTERA Environmental Consultants, Inc., Houston, Texas, for Sandia National Laboratories, 771-00G-05 (1981). Also published in *Groundwater*, 20(5):569-576 (1982).

Sykes, J.F., et al., *Numerical Simulation of Flow and Contaminant Migration at CFB Borden Landfill, Vol. II: Geosphere Transport Model Validation*, prepared by INTERA Environmental Consultants, Inc., Houston, Texas, for Sandia National Laboratories, 771-00G-04 (1981).

Ward, D.S., et al., *Geosphere Model Validation, Vol. I: Verification of the Simulator for Waste, Energy, and Nuclide Transport*, prepared by INTERA Environmental Consultants, Inc., Houston, Texas, for Sandia National Laboratories (1981).

3.22 TEMP: MODIFIED STANFORD FINITE-LENGTH LINE SOURCE CODE

3.22.1 Code Description

TEMP is a three-dimensional code that calculates temperatures generated by finite-length line sources of heat embedded in a geologic medium. The original TEMP code (Kaiser Engineers, 1980) uses a numerical solution to the heat flow equation. The code was then modified by Wurm et al. (1981) to include an analytic solution as an option. The latter report describes only the modification and not the original TEMP code. The TEMP code, in both the modified and original forms, assumes isotropic thermal conductivity and constant thermal conductivity, rock density, and heat capacity throughout an infinite volume.

The numerical solution procedure in TEMP consists of: (1) obtaining the analytic solution (consisting of an integral over time) to the heat flow equation for a line source of finite length, with the source a function of time; (2) dividing the interval of integration into four subintervals; (3) applying the numerical technique of Romberg integration to each of the four subintervals; (4) summing up the integrations over the four subintervals to obtain the temperature increment at an observation point from a single finite-length line source; and (5) summing up the increments from all of the appropriate line sources in the array.

In the modified TEMP code, the numerical solution procedure must be used to find the temperature contributions from finite-length line sources within a certain cutoff distance from the observation point, usually a distance of about 46 meters. The cutoff distance is that distance beyond which the finite line source (waste package) looks like a point source to a temperature sensor. Then, either the numerical or analytic solution procedure can be used for distances greater than the cutoff distance. The analytic solution to the heat flow equation assumes a point heat source, with the source a function of time, and sums the temperature contributions from all the sources beyond the cutoff distance. This procedure was incorporated into TEMP to reduce computing time without sacrificing accuracy.

Input consists of system geometry; thermal conductivity, heat capacity, and density of the geologic medium; time dependence of the heat sources; times at which the heat sources are emplaced; and initial temperature. Output consists of temperature as a function of three spatial dimensions and time.

Limitations of the modified TEMP code include: (1) it assumes constant thermal conductivity and thermal diffusivity throughout an infinite homogeneous medium, thus ignoring the significant inhomogeneity introduced by the repository chambers; (2) thermal conductivity is taken to be independent of temperature; and (3) radiative and convective heat transfer are taken to be negligible. The modified TEMP code is written in FORTRAN and can be run on either a CDC or a VAX computer.

3.22.2 Development Stage

The modified TEMP code is operational on CDC and VAX computers.

3.22.3 Documentation

The documentation in Wurm et al. (1981) is very incomplete and not in the NUREG-0856 (Silling, 1983) format; that is, (1) there is no standard software summary; (2) the problem being solved is not well described; (3) the numerical procedure is not described; (4) there is no discussion of assumptions and limitations; (5) variables are defined, but their dimensions are not presented; (6) the analytic solution is not derived; (7) there is no user's manual; (8) there is no discussion of verification and validation; (9) there is no chronology of versions of the code; and (10) there is no description of a code maintenance and quality assurance program.

Kaiser Engineers (1980, ONWI-94) is well written and relatively complete, but it departs from the NUREG-0856 format in that (1) it has no standard software summary, (2) there is no discussion of assumptions and limitations, (3) validation is not discussed, (4) there is no chronology of versions of the code, and (5) there is no description of a maintenance and quality assurance program.

3.22.4 Performance Specification Review

No external performance specification review has been documented.

3.22.5 Code Design Review

No external code design review has been documented.

3.22.6 Verification

Verification studies were not reported in Wurm et al. (1981). One benchmarking test is reported in ONWI-94 -- a comparison of salt temperatures calculated by TEMP and HEATING5. Agreement was within approximately 10%. Other comparisons, not reviewed by Argonne, appear in McNulty (1983) and McSweeney (1983).

3.22.7 Validation

Validation studies were not reported in Wurm et al. (1981) or in ONWI-94.

3.22.8 Proposed ONWI Application

The modified TEMP code is intended for repository assessment. It can be used to predict temperatures in different geologic media and to find an optimal configuration of waste packages (vertical or horizontal canister emplacement and spacing).

3.22.9 Relationship of Model to Other Codes

The modified TEMP code is basically a stand-alone code. However, its output temperatures, appropriately adapted, should be usable as input to temperature-effects codes like SPECTROM-58, SALT4, or VISCOT.

3.22.10 Application of Code to Other Problems

No other applications of TEMP are known.

3.22.11 Suitability of Model for Salt Repository Application

Several problem areas that could be addressed by TEMP include (1) the possibility of radiative heat transfer in salt (salt is transparent in the infrared), (2) the possible temperature dependence of thermal conductivity, and (3) the inhomogeneity of thermal properties in the vicinity of the repository.

3.22.12 Peer Review

No peer review has been conducted.

3.22.13 References for Section 3.22

Kaiser Engineers, Inc., *Finite-Length Line Source Superposition Model (FLLSSM)*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-94 (March 1980).

McNulty, E.G., *Comparison of TEMPV4 Results with Those Published in Westinghouse AESD-TM3-3131*, Office of Nuclear Waste Isolation letter to G.E. Raines, Battelle Memorial Institute, Columbus, Ohio (April 11, 1983).

McSweeney, T.I., *Comparison of TEMPV3 with Infinite Line Source Analytical Solution*, Office of Nuclear Waste Isolation letter to P. Hofmann, Battelle Memorial Institute, Columbus, Ohio (March 4, 1983).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

Wurm, K.J., et al., *Modification of the TEMP Computer Code — FY 81*, Battelle Memorial Institute, Columbus, Ohio, SPAC-25 (Sept. 1981).

3.23 THAC-SIP-3D: A THREE-DIMENSIONAL TRANSIENT HEAT ANALYSIS CODE USING THE STRONGLY IMPLICIT PROCEDURE

3.23.1 Code Description

THAC-SIP-3D (Turner, 1978) is a general purpose code for solving time-dependent heat transfer problems in a three-dimensional Cartesian coordinate system. The governing equation is the parabolic partial differential equation for heat conduction in solids. (Heat transport by fluid flow is not included.) This equation relates the time rate of change of the temperature to the divergence of the heat flux and the heat generation rate. The input parameters incorporated into the governing equation are thermal conductivity, density, specific heat, and heat generation rate. These parameters will depend on position, temperature, and time; thermal conductivity may be anisotropic. The input parameters can be specified at the boundaries as follows: temperature can be time-dependent, whereas the others can depend on position, temperature, and time.

A finite-difference scheme is used to form a system of algebraic equations that is solved by an iterative procedure called the Strongly Implicit Procedure to obtain the transient temperature distribution. The finite-difference scheme can vary from the Crank-Nicolson to the Classical Implicit Procedure, depending on the value of an input parameter. The scheme is supposed to be fast and accurate, and the convergence rate is not strongly sensitive to the coefficient matrix.

The code output includes maps of temperature distributions for a sequence of planes perpendicular to a user-specified axis. The temperatures are specified at nodes within each plane. The nodal planes need not be orthogonal to the chosen axis.

The code was written in FORTRAN IV for an IBM machine. Core requirements vary from 240K for one temperature node to 1500K for 5000 nodes.

3.23.2 Development Stage

THAC-SIP-3D is a fully operational code. As noted in Turner (1978), it is an updated version of an earlier code developed about five years ago for thermal analysis of waste storage problems. New features include improved input/output characteristics, convective and radiative boundary conditions, enhanced capability to handle temperature dependence, internal adjustment of time-step size, more general convergence criteria, and greater running efficiency.

3.23.3 Documentation

The code is documented in Turner (1978), which deviates from the NUREG-0856 (Silling, 1983) guidelines in two respects: neither a standard software summary nor a user's manual is included. However, Secs. 3 and 4, together with the appendixes, contain all of the necessary ingredients for a user's manual.

3.23.4 Performance Specification Review

No performance specification review has been documented.

3.23.5 Code Design Review

No code design review has been documented.

3.23.6 Verification

Verification of the THAC-SIP-3D code has not been documented.

3.23.7 Validation

Validation of the THAC-SIP-3D code has not been documented.

3.23.8 Proposed ONWI Application

ONWI has not indicated possible applications for THAC-SIP-3D. However, Turner (1978) indicates that this general purpose code could be used for analyzing heat transfer within a waste repository of arbitrary configuration prior to saturation. It could also be used to examine the effects of noncylindrically symmetric distributions of heat sources (waste packages).

3.23.9 Relationship of Model to Other Codes

THAC-SIP-3D is a stand-alone code, but it could be used in conjunction with less sophisticated models, such as the thermal process model in the WAPPA package that requires cylindrical symmetry. This code could also be used to assist in determining proper thermal boundary conditions at the waste-package/repository interface for use by other codes that include coupling of heat transport to other physical and chemical processes. THAC-SIP-3D is similar, but not identical, to HEATING6.

3.23.10 Application of Code to Other Problems

Applications to other problems have not been documented.

3.23.11 Suitability of Model for Salt Repository Application

The suitability of THAC-SIP-3D for salt repository applications has not been addressed in the documentation. However, given the generality of the code, it would be suited to salt repository applications in which dry heat transport is the only issue. Coupling to such processes as energy transport by fluid flow cannot be considered for this code.

3.23.12 Peer Review

THAC-SID-3D has not been subjected to peer review.

3.23.13 References for Section 3.23

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

Turner, W.D., *THAC-SIP-3D: A Three-Dimensional, Transient Heat Analysis Code Using the Strongly Implicit Procedure*, Oak Ridge Gaseous Diffusion Plant, Oak Ridge, Tenn., K/CSD/TM-24 (Sept. 1978).

3.24 TRIPM: A TWO-DIMENSIONAL FINITE-ELEMENT MODEL FOR THE SIMULTANEOUS TRANSPORT OF WATER AND REACTING SOLUTES THROUGH SATURATED AND UNSATURATED POROUS MEDIA

3.24.1 Code Description

TRIPM (Gureghian, 1983, ONWI-465) simulates transport in two dimensions of aqueous solutions of chemically active and radioactive contaminants in saturated and unsaturated porous media. The code can handle formation and decay of species in a decay chain, first-order chemical activity, and reversible adsorption onto the porous media. It accounts for the effects of soil and water pH on the distribution coefficient that relates the concentration of the contaminant adsorbed on the porous media to that in solution.

The code consists of two separate parts, one that calculates the pressure distribution in the geologic region of interest and one that calculates the migration of various contaminants through the porous media. The finite-element method is based on the weighted-residual technique. The principal model equations, namely the flow and

solute concentration equations, are solved by the Bubnov-Galerkin and Petrov-Galerkin methods, respectively. Both quadrilateral and triangular elements can be used.

The model was designed primarily as a tool for evaluating the capacity of the unsaturated zone of unconfined aquifers to act as a natural barrier to transport to groundwater of radionuclides leached from uranium mill tailings; shallow land-burial sites; or solid, low-level radioactive wastes. It is written in FORTRAN IV and has been run on an IBM 370-195 machine.

3.24.2 Development Stage

The code is operational and is available, along with documentation, from ONWI and from the National Energy Software Center. It is a new code that has undergone little testing or field application.

3.24.3 Documentation

TRIPM is documented in ONWI-465, but the documentation does not conform in several important ways to NUREG-0856 (Silling, 1983). First, although the theory and solution method are described in detail, the range of applicability is not discussed at all. Second, the input requirements and output options are not clearly summarized. While it is evident from the example problems that the flow domain may consist of several separate subdomains, each containing different soil types, it is not clear what the constraints are. Must these subdomains be homogeneous and isotropic? Must they have uniform temperatures? How many layers are permitted? Third, there is no user's manual and no code listing. Several test problems are briefly described with good graphics, but it is not clear whether these test problems constitute code verification, model validation, or sensitivity analysis, or whether they are just illustrative examples. Finally, it is not obvious how the various reactions, reactants, and processes are entered into the code, nor is it evident how many processes and species can be treated simultaneously.

3.24.4 Performance Specification Review

No internal or external performance specification reviews have been documented.

3.24.5 Code Design Review

No internal or external code design reviews have been documented.

3.24.6 Verification

ONWI-465 briefly describes six problems that were run. Two were one-dimensional problems and four were two-dimensional. All involved near-surface aquifers.

1. One-dimensional code verification; multisolute solution transport with first-order reactions. This problem involved movement of NH_4^+ , with nitrification and a linear equilibrium isotherm in a saturated soil column and no adsorption. Comparison of concentration profiles of three species obtained using both the Bubnov-Galerkin and Petrov-Galerkin numerical schemes with a published analytical solution showed very good agreement for simulation times up to 100 days.
2. One-dimensional model validation; transport of an aqueous solution of a conservative ionic species (Cl^-) in an unsaturated, homogeneous soil. The soil moisture content profile after two- and nine-hour infiltrations compared well with experimental observations. The concentration profile comparison was not as good. The general profile shape was satisfactory, but it exhibited a significant time lag. Results proved to be somewhat sensitive to choice of boundary conditions.
3. Two-dimensional model validation test; transient water-table recharge. This problem involved a near-surface aquifer with a drainage ditch. Comparison of the calculated and observed water-table position as a function of time showed reasonable agreement for a test period of four hours.
4. Two-dimensional model validation test; transient falling water table. This problem also involved a near-surface aquifer with a drainage ditch. Comparison of the calculated and observed water-table profiles was satisfactory except near the drainage ditch.
5. Two-dimensional model example problem; ditch-drained aquifer with incident steady rainfall and trickle infiltration of Cl^- . The results for two alternative choices of boundary conditions were compared. Differences were evident but not discussed.
6. Two-dimensional model example problem; transport of a three-membered radioactive decay chain. This problem involved a pit used to store radioactive liquid waste, with steady state infiltration of water into an aquifer. The discharge rate of radioactive-bearing solution was constant for the first 10 years of simulation time but declined over next 10-year simulation period. The flow regime included three soil types. Both quadrilateral and triangular elements were used in integration.

Of the above six tests, one constituted a one-dimensional code verification test, one constituted a one-dimensional code validation test for up to nine hours of simulation time, and two constituted two-dimensional code validation tests. In view of the capabilities of this model to simulate several processes, it cannot be said to be fully verified.

3.24.7 Validation

The only validation reports are those described in Sec. 3.24.6 as tests 2, 3, and 4, which are described in more detail in ONWI-465. These three tests compare calculations with experimental results for rather idealized aquifers for periods of several hours of experimental and simulation time.

3.24.8 Proposed ONWI Application

On the basis of its design for use in near-surface aquifer analysis, TRIPM would presumably be useful for far-field applications involving infiltration of contaminated water carrying leachates from breached waste packages into either saturated or unsaturated aquifers. The code's applicability to deep aquifers is not obvious from the documentation.

3.24.9 Relationship of Model to Other Codes

While TRIPM can be operated as an independent model of transport of contaminated aqueous solutions in aquifers, it must be coupled to other codes and data bases if it is to be meaningful in the repository assessment process. In particular, TRIPM requires information on solution speciation and on the physical and chemical properties of the porous media constituting the aquifers of interest, as well as on the boundary conditions. Several iterations between TRIPM and the other transport and source codes would probably be required to properly establish the boundary conditions. Solution speciation, in particular, would have to be obtained from source, geochemistry, and near-field transport codes like ORIGEN2, WAPPA, and EQ3/EQ6, and then combined with applicable hydrological transport codes.

3.24.10 Application of Code to Other Problems

ONWI-465 describes applications of TRIPM to the six different problems briefly summarized in Sec. 3.24.6. All involved movement of aqueous solutions in near-surface aquifers. One problem involved three radioactive decay-chain species and sought to measure the effects of adsorption on the porous media. Another involved three chemically active species. U.S. Nuclear Regulatory Commission (1980) describes the Gas Hills Uranium Project, which used the TRIPM code.

3.24.11 Suitability of Model for Salt Repository Applications

It is not possible to judge TRIPM's suitability for salt repository applications without more detailed information. The code documentation does not indicate whether the code is applicable to deep aquifers and to highly concentrated brine solutions. However, it does appear to be suitable for dilute solutions of radioactive and chemically reactive species in near-surface aquifers. Ranges of applicability as far as temperature and pressure (and their gradients) and solute concentrations are not given.

3.24.12 Peer Review

No peer reviews of the TRIPM code have been documented.

3.24.13 References for Section 3.24

Gureghian, A.B., *TRIPM: A Two-Dimensional Finite-Element Model for the Simultaneous Transport of Water and Reacting Solutes through Saturated and Unsaturated Porous Media*, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-465 (June 1983).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

U.S. Nuclear Regulatory Commission, *Final Environmental Impact Statement: Gas Hills Uranium Mill, Union Carbide Corporation, Natrona County, Wyoming*, NUREG-0702 (1980).

3.25 UCB-NE-n: MIGRATION OF RADIONUCLIDES THROUGH SORBING MEDIA

3.25.1 Code Description

This set of UCB-NE-n ($n = 2, 10, 25, 30, 40, 50$, and 60) codes (Harada et al., 1980, ONWI-359; Pigford et al., 1980, ONWI-360) models the transport in groundwater of radionuclides belonging to radioactive decay chains through fully saturated, porous, sorbing geologic media. The different codes (1) correspond to fluid flow in one- and two-dimensional flow fields; (2) provide for a single chemical state or various different chemical species of a radionuclide; (3) permit different assumptions regarding parameters, such as rates of dissolution and solubility limits; and (4) deal with different boundary conditions.

The UCB-NE-n codes originated from studies on the migration of radionuclides through sorbing media conducted at the University of California, Berkeley, and the Department of Nuclear Engineering and the Earth Sciences Division of Lawrence Berkeley Laboratory (Harada et al., 1980; Pigford et al., 1980). The codes provide analytical or semianalytical solutions of mass transport equations for radionuclides in a decay chain. As elaborated in Table 4, the various codes solve transient mass transport equations with varying dimensionality, speciation, phenomenology, and boundary conditions.

In ONWI-359, basic transport equations are derived that describe the space-dependent and time-dependent concentration of a radionuclide in groundwater as the radionuclide propagates by convection and dispersion through a geologic porous medium, with sorption occurring between the solid and liquid. The equations are formulated for a radionuclide member of a radioactive decay chain of arbitrary length. Boundary

TABLE 4 Radionuclide Transport Model Characteristics in the UCB-NE-n Code Series^{a,b}

Characteristic	n=10	n=25	n=30	n=40	n=50	n=60
Closed-form analytical solution	Yes	Yes	Yes	Yes	Yes	Yes
Radioactive chain decay	Yes	Yes	Yes	Yes	Yes	No
Dimension of mass transport equation	1	1	1	2	2	1
Dimension of flow field	1	1	1	1	2	1
Steady flow	Yes	Yes	Yes	Yes	Yes	Yes
Homogeneous or layered medium	Homogeneous	Homogeneous	Layered	Homogeneous	Homogeneous	J
Single or multiple chemical species	Multiple					
Source release rate	A or C	A	A or B	A	A	A
Solubility limit at source	D					D
Source configuration				E or F, or G or H		
Equilibrium sorption	Yes	Yes	Yes	Yes	Yes	Yes
Finite rate absorption			Yes			
Equilibrium fluid-phase chemical reactions	Yes					
Nuclide solubility	Yes					Yes

- ^aA - constant over finite time period,
 B - geometrically controlled variable,
 C - other,
 D - for first member of decay chain only,
 E - single point source,
 F - array of point sources,
 G - single finite plane source,
 H - array of finite plane sources,
 J - fracture and bulk medium are homogeneous, and
 No entry - information not immediately available.

^bNo data were found for n = 2.

conditions reflect the time-dependent dissolution rate of a particular radionuclide into groundwater at the point where the waste is emplaced in a geologic repository.

Analytical solutions presented in ONWI-359 are for one-dimensional transport with local chemical and sorptive equilibrium. These solutions are presented both in a recursive form and also in a general explicit form. The explicit solution in the absence of dispersion is presented for a radionuclide in a decay chain of arbitrary length. Solutions are presented for migration in an infinite homogeneous porous medium as well as in layered porous media. The general solutions in ONWI-359 were used extensively in developing the new analytical solutions presented in ONWI-360.

In ONWI-360, solutions are generated for one-dimensional equilibrium transport in an infinite medium. The explicit solution for a radionuclide in a decay chain of arbitrary length, presented in ONWI-359 for no dispersion, is extended in ONWI-360 to include dispersion. These solutions are also extended to include the effect of possible irreversible mineralization of sorbed radionuclides.

Analyses in ONWI-359 assume the dissolution of an infinite plane source of radionuclides, and the demonstrations assume either a constant fractional rate of dissolution of contained radionuclides or a constant rate of dissolution of the waste matrix. In ONWI-360, the time-dependent dissolution rates for specific canister geometries are developed for equivalent planar sources.

In ONWI-360, the solutions for one-dimensional equilibrium transport in multi-layered media are applied to calculate the transport of ^{237}Np through a specially sorbing overpack surrounding a waste canister, followed by its transport into the surrounding geologic medium.

Solutions in ONWI-359 assume that there is no solubility limit on the concentration of a radionuclide in groundwater. In ONWI-360, these equations are modified to calculate the solubility-limited transport of a radionuclide with no precursors, assuming that the radionuclide is released from the waste when the waste matrix dissolves. The solution is then applied to calculate the solubility-limited transport of ^{239}Pu in a geologic medium, assuming dissolution of waste canisters containing unprocessed spent fuel and other canisters containing highly radioactive reprocessed glass waste.

The ONWI-359 analyses assume that a given radionuclide exists in a single chemical state in the liquid and in a single sorbed state on the solid. In ONWI-360, the possibility of several different chemical states (e.g., oxidation states, complexes, and polymers) or a radionuclide in the liquid and on the solid is considered, with the assumption of local chemical equilibrium.

ONWI-360 extends the analytical solutions of one-dimensional transport to include the departure from local chemical equilibrium. Of possible importance for long-term migration in some geologic media and of likely importance in some laboratory and field experiments is the transport of a dissolved radionuclide that has not reached sorption equilibrium with the adjacent solid. These nonequilibrium effects are important in deducing sorption mechanisms from laboratory and field data, and they may contribute to accelerated transport of some radionuclides.

Another nonequilibrium phenomenon considered in ONWI-360 is the possible nonequilibrium reversible mineralization of a portion of the sorbed radionuclides, which can alter both the magnitude and shape of the concentration profile of this radionuclide as it propagates through the geologic medium. The effects of nonequilibrium mass transfer between liquid and solid, and nonequilibrium reversible mineralization reactions, are included in a new analysis of nonequilibrium transport in a one-dimensional flow field, an analysis that is applicable to a radionuclide in a multimember decay chain.

A third nonequilibrium phenomenon considered is the existence of two or more chemical species of a dissolved radionuclide, with these species related to each other by rate processes rather than by simple equilibria. New analytical solutions for these nonequilibrium effects are presented in ONWI-360.

In the one-dimensional solutions presented in ONWI-359, dispersion is assumed to occur only in the direction of the one-dimensional flow of groundwater. This is a proper condition for one-dimensional convective transport of radionuclides dissolved from an infinite plane source. However, before applying these results to discrete waste sources or to repository emplacements of finite size, the effects of transverse dispersion must be incorporated. In ONWI-360, new analytical solutions are presented for the space-time-dependent concentration of a radionuclide in a decay chain of arbitrary length. These solutions assume a time-dependent point source, one-dimensional flow of groundwater, and local chemical equilibrium between the groundwater and the adjacent solid.

Although the analytical solutions for one-dimensional groundwater flow are useful for establishing benchmarks for numerical solutions and for some long-term predictions of radionuclide transport, full utilization of the power of analytical solutions for benchmark and predictive purposes does not obtain until solutions for radionuclide transport in two-dimensional and three-dimensional flow fields are developed. The new solutions for multidimensional radionuclide transport presented in ONWI-360 are derived for the time-independent, incompressible, multidimensional flow of groundwater through porous media. Solutions have been obtained in both the recursive and the general explicit form for a radionuclide in a decay chain of arbitrary length, with local chemical equilibrium between the water and solid. These solutions provide a useful tool for predicting radionuclide transport along a hydrologic flow field that has been established from field data or from hydrologic mapping.

As a departure from analytical solutions of the basic transport equations, finite-element solutions of one-dimensional and two-dimensional transport of radionuclides through porous media, with one-dimensional flow of groundwater, are presented in ONWI-360, with the results being compared with those of the analytical solutions. (The finite-element numerical technique can also be applied to multilayered media.) Finite-element analysis is an alternate approach to the solution of the basic transport equations and compares favorably with the numerical solution of the partial differential equations as used in existing numerical codes.

Input to a member of this code set would include the following data as a composite example (with some variation from code to code, depending on code characteristics as specified in Table 4): names and half-lives of the nuclides and their hierarchy in a radioactive chain, initial nuclide inventory, retardation factors, solubility limits,

reaction equilibrium coefficients, release rate at the source, time of initial release, dispersion coefficients, water velocity, water volumetric flow rate, rock porosity, and fracture width and length, if applicable.

The output from a member of this code set would include the following data as a composite example (with some variation from code to code, depending on code characteristics): names of the nuclides, time after emplacement, distance from the repository, discharge rates of the nuclides (in a fracture, if applicable), and aqueous concentration of nuclides in the rock. In some code formats, different presentations of essentially equivalent information are supplied.

Certain of these codes are referred to by alternate designations in the literature. For example, computer code UCB-NE-10 is also referred to as MGRAT03, and computer code UCB-NE-25 is also referred to as MAX 1.

No summary of model classes for the codes in this set is available. As an example of model complexity, however, the computer code UCB-NE-10 consists of a main program, five subprograms, and four function programs, with a total of about 600 lines of instruction. FORTRAN IV is used for UCB-NE-10, while FORTRAN is used for UCB-NE-25. Code UCB-NE-10 was written for the CDC-6600/7600 computer. Information on storage requirements and running times is not readily available for these codes.

3.25.2 Development Stage

Some of the UCB-NE-n codes (e.g., UCB-NE-10 and UCB-NE-25) appear to be ready for use.

3.25.3 Documentation

Although the theory and solution techniques have been well documented in ONWI-359 and ONWI-360, documentation of the codes is incomplete and inadequate. Documentation and users' manuals meeting NUREG-0856 (Silling, 1983) requirements do not exist. It appears that ONWI plans to use the code set primarily to verify other codes using numerical solution techniques. However, if a particular UCB-NE-n code should be chosen for performance assessment, it would need to be redocumented according to NRC requirements (ONWI, 1983a).

3.25.4 Performance Specification Review

ONWI (1983a) reports that internal review was completed and that no external review is planned.

3.25.5 Code Design Review

ONWI (1983a) reports that internal review was completed and that no external review is planned.

3.25.6 Verification

Various analytical solutions (e.g., three-dimensional versus one-dimensional models) were compared and verified against each other. In addition, the finite-element numerical technique was used, and the results of finite-element solutions of the transport of a three-member decay chain of radionuclides ($^{234}\text{U} + ^{230}\text{Th} + ^{226}\text{Ra}$) in a one-dimensional flow of groundwater were compared with analytical solutions. These comparisons are reported in detail in ONWI-359 and ONWI-360.

ONWI (1983a) reports that the UCB-NE-n codes were adequately compared against other computer codes using test cases from the six benchmark problems presented at the INTRACON meeting held in February 1982 in Switzerland (Jansen and Hewitt, 1982; Grundfelt and Anderson, 1983).

UCB-NE-n codes were used in test cases for verification of the radionuclide transport analysis code LAYFLO. These cases involved calculations of the one-dimensional transport of radionuclides in three-member decay chains (Gureghian and Jansen, 1983). Code UCB-NE-25 was used for calculating discharge concentrations of ^{234}U , ^{230}Th , and ^{226}Ra in the radioactive decay chain $^{234}\text{U} + ^{230}\text{Th} + ^{226}\text{Ra}$ for the nondispersive case in a homogeneous (one-layer) medium, and the results were compared with those calculated using LAYFLO. The agreement in the results was excellent. Code UCB-NE-10.2 was used for the nuclides of the same decay chain for the advective-dispersive case in a homogeneous (one-layer) medium and the results compared with those from LAYFLO. Agreement was again excellent. The case of advection in a two-layer medium was examined with two test problems of different three-member decay chains, $^{234}\text{U} + ^{230}\text{Th} + ^{226}\text{Ra}$ and $^{245}\text{Cm} + ^{237}\text{Np} + ^{233}\text{U}$. UCB-NE-30 and LAYFLO results were compared, and they seemed to agree exactly.

3.25.7 Validation

The UCB-NE-n code set has not been validated, and no validation is planned at this time. However, if a particular code should be selected for performance assessment, it would be validated with site-specific data obtained from site characterization (ONWI, 1983a).

3.25.8 Proposed ONWI Application

The UCB-NE-n codes are included among the site assessment codes for salt repositories (ONWI, 1983b). ONWI plans to use them primarily to verify other codes using numerical solution techniques (ONWI, 1983a).

3.25.9 Relationship of Model to Other Codes

Many other radionuclide transport codes exist. In Science Applications (1981) and Thomas et al. (1982) are tabulations of geosphere solute transport codes, in particular, subsurface hydrological models, including groundwater flow and nuclide transport codes. MMT, LAYFLO, GETOUT, and MIGRAIN are examples of related programs.

3.25.10 Application of Code to Other Problems

No applications of the UCB-NE-n codes to other problems have been identified. These models and codes were developed specifically for ONWI and have been applied to examples relevant to transport in groundwater of radionuclides from nuclear waste.

3.25.11 Suitability of Model for Salt Repository Application

The models on which these codes are based were developed specifically for ONWI for applications to transport in groundwater of radionuclides from nuclear waste. An example of a salt-specific limitation is that dissolution of salt would complicate transport (density driven flow) and absorption.

3.25.12 Peer Review

No peer review of UCB-NE-n is planned unless the code is selected for repository performance assessment (Office of Nuclear Waste Isolation, 1983a).

3.25.13 References for Section 3.5

Grundfelt, B., and K. Anderson, *INTRACOIN — Report of Final Results of Level 1, International Nuclide Transport Code Intercomparison Study* (1983).

Gureghian, A.B., and G. Jansen, *LAYFLO: A One-Dimensional Semianalytical Model for the Migration of a Three-Member Decay Chain in a Multilayered Geologic Medium*, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-466 (May 1983).

Harada, M., et al., *Migration of Radionuclides through Sorbing Media, Analytical Solutions I*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, by Lawrence Berkeley Laboratory, ONWI-359 (1980).

Jansen, G., and W. Hewitt, *Foreign Trip Report, INTRACOIN, International Nuclide Transport Code Intercomparison Study Workshop and Coordinating Committee Meeting, Interlaken, Switzerland, Feb. 15-20, 1982*, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio (Sept. 1982).

Office of Nuclear Waste Isolation, *Verification and Validation Plan for Performance Assessment Technology for a Nuclear Waste Repository in Salt*, Battelle Memorial Institute, Columbus, Ohio, unpublished manuscript (1983a).

Office of Nuclear Waste Isolation, *Preliminary Performance Assessment Plan for a Nuclear Waste Repository in Salt*, Battelle Memorial Institute, Columbus, Ohio, unpublished manuscript (1983b).

Pigford, T.H., et al., *Migration of Radionuclides through Sorbing Media, Analytical Solutions II*, Vols. I and II, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, by Lawrence Berkeley Laboratory, ONWI-360(1) and ONWI-360(2) (Oct. 1980).

Science Applications, Inc., *Tabulation of Waste Isolation Computer Models*, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-78 (Aug. 1981).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

Thomas, S.D., et al., *A Summary of Repository Siting Models*, prepared for U.S. Nuclear Regulatory Commission, NUREG/CR-2782 (July 1982).

3.26 VISCOT: A TWO-DIMENSIONAL AND AXISYMMETRIC NONLINEAR TRANSIENT THERMOVISCOELASTIC AND THERMOVISCOPLASTIC FINITE-ELEMENT CODE FOR MODELING TIME-DEPENDENT VISCOUS MECHANICAL BEHAVIOR OF A ROCK MASS

3.26.1 Code Description

VISCOT (INTERA, 1983, ONWI-437) is a two-dimensional (planar or axisymmetric) finite-element code for calculating time-dependent, nonlinear deformations of a rock mass in response to geostatic and thermal stresses. The rock mass is modeled as viscoelastic or viscoplastic. Input consists of a description of the geometry of the physical system being modeled, initial and boundary conditions, material properties (Young's modulus, Poisson's ratio, coefficient of thermal expansion, mass density, and other parameters used in modeling the rock mass), and temperatures at the nodes. In the transient case, the nodal temperatures are specified at successive times. Output consists of the predicted displacements, stresses, and strains, plus a summary of the input data.

VISCOT uses a Bubnov-Galerkin finite-element technique with an explicit Euler time-stepping scheme to solve a system of equations consisting of the force equilibrium equation, the stress-strain relation, and the equations that describe the viscoelastic or viscoplastic deformation. It is restricted to simulating systems that are either two-dimensional planar or axially symmetric. Additional limitations are: (1) mechanical and thermal properties must be isotropic, (2) the rock mass is treated as a continuum (i.e., VISCOT is inapplicable when there is significant fracturing), (3) large deformations cannot be accurately simulated, and (4) it is possible to obtain the input temperatures from the DOT code only when both DOT and VISCOT employ identical mesh geometries. VISCOT is written in FORTRAN IV for use on a CDC CYBER 176 computer.

3.26.2 Development Stage

VISCOT is ready for use.

3.26.3 Documentation

Although the code documentation in ONWI-437 is in the NUREG-0856 (Silling, 1983) format and is generally quite good, it has one major inadequacy plus a number of minor deficiencies. The major inadequacy is that ONWI-437 does very little to help the user develop an intuitive physical understanding about the kinds of processes simulated by the model. The user needs such an understanding to provide appropriate input to and to interpret output from VISCOT.

If the necessary physical understanding can be attained by reading certain background references, then ONWI-437 should make that clear and direct the reader to those texts. For example, a reference is needed to a text that explains how one distinguishes between thermal strain and inelastic strain (p. 10).^{*} Otherwise, ONWI-437 should itself present material, like the example suggested below, that would help the reader develop the necessary understanding. In addition to defining the terms "viscoelastic," "viscoplastic," and "elastoplastic," examples should be presented to help the reader understand the physics behind the mathematical formalism. One possibility is a two-dimensional, rectangular, vertical column subject to loading. The column could be taken to represent a rock mass that is linearly elastic, then one that is viscoelastic, and finally one that is viscoplastic. The effects of geostatic stresses alone, thermal stresses alone, and then both together could be demonstrated.

The problems solved in Sec. 4 (Verification Test and Results) constitute examples, but they are only slightly helpful. For example, in the comparison between the analytic and VISCOT solutions in the case of the one-dimensional viscoelastic bar (pp. 34-41), it is not clear on pages 36-37 whether Fig. 4-2a shows Case 1 and Fig. 4-2b shows Case 2, or vice versa. Further, the text on page 36 refers to "nodes 1 and 2 depicted in Figure 4-2a," but there are no numbered nodes shown in that figure. Also, the boundary condition notation is not explained for either figure. Finally, what is the physical explanation for the difference in behavior between cases 1 and 2 (see Fig. 4-3)? The viscoplastic thick cylinder problem discussed on pages 42-48 in Sec. 4 is also confusing. Pressure is listed on page 43 as having the value 14 dyne/mm² on the interior surface of the cylinder, but the text on page 42 states that the pressure is gradually increasing. Also, what is the pressure on the cylinder's outer surface?

Other but minor deficiencies in documentation are:

1. The applicability of VISCOT to a salt repository is insufficiently discussed. For example, are the mechanical and thermal properties of salt isotropic?

^{*}Page numbers in Sec. 3.26 are from ONWI-437.

2. It is ambiguous to state that "the deformations and strains within the rock mass are either two-dimensional or axisymmetric and small" (p. 19). Further, it is not clear what is meant by "small."
3. The results of the verification tests should be summarized and an overall conclusion drawn.

3.26.4 Performance Specification Review

An internal review of the first draft of ONWI-437 has been completed by INTERA and ONWI. No external review is documented.

3.26.5 Code Design Review

The statement in Sec. 3.26.4 applies here as well.

3.26.6 Verification

ONWI-437 describes five VISCOT verification tests -- four involving comparisons with analytic solutions and one with the results of an alternative computational procedure. In all but one of the four comparisons with analytic solutions, VISCOT performed well. However, in the case of a rectangular plate subject to a parabolic temperature distribution (p. 49), VISCOT did not do well. Specifically, Table 4-3 (p. 52) shows that:

1. One VISCOT output value for the stress component σ_{xx} was +6.8311, while the corresponding analytic value was -6.7537. This discrepancy may be a typographical error.
2. A second value for σ_{xx} produced by VISCOT is 2.4450, while the corresponding analytic value is -6.7551. This represents a greater than 100% difference.
3. The last two σ_{xx} VISCOT values in the table (-0.3221 and -0.3791) differ from the corresponding analytic values (0.7862 and 0.7862) by more than 100%. Nonetheless, the text describes the VISCOT and analytic values as being "in good agreement" (p. 49). While this is true for most of the corresponding values listed in Table 4-3, it is not true for all.

3.26.7 Validation

The VISCOT code has not been validated.

3.26.8 Proposed ONWI Application

VISCOT will be used for repository assessment. It can do room-scale calculations to generate input for predicting rates of room-closure, stability, and floor heave in rock masses. It can also calculate the stress within the backfill material.

3.26.9 Relationship of Model to Other Codes

To accomplish a complete thermomechanical analysis, a SCEPTER thermal analysis code (e.g., DOT) must be used to provide input temperatures to VISCOT. If DOT is coupled with VISCOT, both must use the same mesh geometry.

3.26.10 Application of Code to Other Problems

No other applications of VISCOT are known.

3.26.11 Suitability of Model for Salt Repository Application

The following limitations will need to be taken into account in applying VISCOT to a salt repository: (1) the model cannot treat three-dimensional deformation, (2) it cannot simulate an anisotropic or fractured material, (3) it assumes small deformations, and (4) the assumptions listed on page 19 may not all be satisfied for salt.

3.26.12 Peer Review

Formal peer review of VISCOT has not been carried out.

3.26.13 References for Section 3.26

INTERA Environmental Consultants, Inc., *VISCOT: A Two-Dimensional and Axisymmetric Nonlinear Transient Thermoviscoelastic and Thermoviscoplastic Finite-Element Code for Modeling Time-Dependent Viscous Mechanical Behavior of a Rock Mass*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-437 (1983).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

3.27 WAPPA: A WASTE PACKAGE PERFORMANCE ASSESSMENT CODE

3.27.1 Code Description

WAPPA (INTERA, 1983, ONWI-452) is designed to evaluate waste package design performance in a repository in a geologic medium. The code determines the integrity of the barriers designed to isolate the waste form from the repository. It computes the heat and radionuclide fluxes at the waste-package/repository interface as a function of time. The code can handle solid waste forms surrounded by up to 17 barriers, including a backfill layer. The waste forms must be homogeneous, brittle, and uniformly leachable. Cladded spent-fuel assemblies and "cermet" waste forms are not accurately treated because of their structural inhomogeneities and deviations from the required cylindrical symmetry.

From a systems point of view, WAPPA transforms output data from codes that provide information on the nuclide inventory and the heat generation rate within a particular waste form as a function of time and from codes that provide information on temperature, mechanical stress, and fluid-flux boundary conditions as a function of time at the waste-package/repository interface into heat and nuclide fluxes at that interface for use by other codes that treat transport in the near field. Although all of the codes involved in this sequence of processing input and output information are operated independently of each other, the waste-package/repository system is naturally coupled. Therefore, the boundary conditions at the waste-package/repository interface cannot be determined in a self-consistent manner without proper treatment of the coupling.

WAPPA assumes cylindrical symmetry, which seems satisfactory for an isolated waste package, but ignores the possibility that the distribution of waste packages within the repository may significantly alter that symmetry. The consequences of this limitation have not been addressed.

The code comprises five process models -- radiation, thermal, mechanical, corrosion, and leaching. The radiation and thermal process models are driven internally from the nuclide inventory and heat generated within the waste form. The corrosion and leaching process models are driven externally by external mechanical stresses and fluid fluxes. Corrosion is treated from the outside inward; that is, corrosion originating internally is not considered. Although corrosion rates can be enhanced by radiation, possible degradation of the mechanical properties of the barrier materials by radiation damage is not treated. The corrosion model begins operation when the user-input data indicate that the backfill has been wetted. In other words, the user must provide a time when the repository becomes saturated. The leach model begins operation when all of the barriers have been breached and fluid from the repository contacts the waste form. The waste form is continuously subject to radiation and mechanical damage.

The code operates over a sequence of up to 30 time steps, covering a geologic period of about one million years. During each time step, the five process models operate independently of each other and degrade the barriers. At the end of each time step, the effects of all of the processes on the barriers are integrated, and the status of all barriers is updated. During the next time step, the process models operate on the

updated barriers. In this way the operation of the process codes is coupled together. A restart option allows the user to add or insert additional time steps to obtain better time resolution.

The radiation process model requires a user-specified data set containing nuclide inventory and heat generation data as a function of time for the specific waste form of interest. These data must be obtained from a detailed code like ORIGEN2 that treats the characteristics of a waste form after irradiation of the waste products. The radiation process model takes data directly from a look-up table, if the time steps are properly chosen (20 for ORIGEN2), or interpolates for other times. Empirical input data are required for gamma ray attenuation by the package components, radiation damage to the waste form, and corrosion and leach enhancement related to radiolysis processes.

The thermal process model treats heat flow across concentric annuli using input from the ORIGEN2 code or its alternatives. The three basic forms of heat transfer are considered.

The mechanical process model calculates radial and axial stresses, and canister and waste form fracturing. Required inputs include state of stress at the waste-package/repository interface and thermal input from the thermal process model. Only tensile-stress fracturing of the waste form is treated.

The corrosion process model comprises five corrosion submodels -- general corrosion, localized pitting and crevice corrosion, stress corrosion, galvanic corrosion, and dry oxidation. Of these, pitting and crevice corrosion and stress corrosion are assumed to be catastrophic. If they are operative for a particular barrier within a given time step, that barrier is assumed to be breached or completely destroyed during that time step. Three important limitations to the corrosion process model are:

1. Internal corrosion is ignored, which may be a nonconservative assumption.
2. Only galvanic corrosion between pairs of metal barriers is considered. Single-barrier galvanic corrosion is ignored, which may be a nonconservative assumption.
3. Effects of corrosion films are ignored, which is presumably a conservative assumption.

The leach process model calculates the mass transport of nuclides across the waste-package/repository interface as a result of both diffusive and advective transport. The backfill is treated by this model as a "mixing cell." In other words, the backfill is assumed to be instantaneously and uniformly wetted by new fluid entering from the repository or contaminated fluid entering from the interior waste package. The boundary condition at the interface is assumed to be of the "swept-away" type; that is, any nuclides crossing the interface are immediately swept away so that no accumulation occurs. No accumulation means that the effluent from one waste package can never influence an adjacent waste package. The consequences of ignoring cumulative effects (nonzero nuclide concentrations in the near field) are not addressed.

Sophisticated numerical methods are not used by any of the process models. Most of them are closed-form analytical expressions requiring empirical input data. The leach model solves four simple simultaneous equations using the Gauss-elimination technique. Further, the model assumes swept-away boundary conditions, so that the concentration of nuclides in the repository at the interface with the waste package is always assumed to be zero.

Written in ANSI-77 FORTRAN, the WAPPA code has been installed on a CDC 7600 machine and consists of approximately 12,000 lines of code. It runs very fast, requiring only a few seconds of CPU time for a fully dimensioned problem. The code provides both summary and detailed outputs, the latter including status of barriers as a function of time, and nuclide concentrations as a function of radius. Tabulations of heat and nuclide fluxes at the waste-package/repository interface are also given.

3.27.2 Development Stage

WAPPA is a fully operational and documented code.

3.27.3 Documentation

The code has been documented in accordance with NUREG-0856 (INTERA, 1983; Silling, 1983). The theory of each of the five process models is explained in detail, as is the verification procedure. A detailed user's manual is provided, along with a code listing on microfiche. The documentation is quite complete, although not without problems. Although the overall structure of the code is clear enough, the interactions among the five independent process models are difficult to unravel. The information is all there, but it tends to be buried in the descriptions of the individual process models. It is not always clear which interactions are included and how they are implemented.

For example, the mechanical model assumes that when the backfill stress limit is exceeded, the backfill "fails" and is thereafter treated as an incompressible fluid. It does not say what happens, if anything, to all of the other properties of the backfill in this "failed" state. The mechanical model also fails to mention the influence of stress on the solubility of the waste form. As another example, emphasis is placed on the need to have more flexibility in the choice of corrosion film growth models. Yet, the user is left in the dark as to how the growth of films influences the outcome of the calculations. In fact, it appears that such films are calculated but that their effects are subsequently ignored.

Although most of the physical processes treated by the five process models are described in ONWI-452, the physical process descriptions are not adequate in many cases to give a clear picture of what is going on. For example, the backfill barrier is described in terms of a "mixed-cell" model in which "new" and "old" fluids are instantaneously mixed. What is presumably meant is that the resistance to flow in the backfill media is much lower than that in the remainder of the waste package so that any deviation from cylindrical symmetry is removed. Still, one is left wondering whether only radial flows are considered or whether more complex flows in the repository are envisioned. Perhaps

the backfill region is intended to serve as a transition from the more complex flow pattern to one of radial flow within the interior waste package.

3.27.4 Performance Specification Review

ONWI-452 lists the performance specifications for WAPPA, but no external review is documented. The documentation lists the assumptions and limitations of each of the process models, as well as of the code verification tests. However, the justification for why certain processes are treated while others are ignored is often missing as illustrated below:

1. On page 15* it states that "the material properties for the Mechanical Model and Leach Model are not assumed to be temperature dependent." This statement deserves both clarification and justification.
2. Both wet and dry corrosion processes are limited to the exterior surfaces of the barriers; that is, corrosion of interior surfaces is not considered. Also, no consideration is given to the formation and transport of gases within the waste form. If these processes are assumed to be negligible compared with the other processes, some justification should be given.
3. On page 38 no justification is given for the statement that "only certain wasteform physical properties are considered to be degraded by radiation [and that] degradation to barrier materials is not considered."
4. On page 80 it states that "the wasteform fractures only under tensile loading." Why are compression fractures ignored?
5. On page 124 it states that "galvanic corrosion due to local cells on one single barrier is not considered in the present model, nor could it be practically modeled." Why? Isn't this a potentially important process?
6. Very little is said about chemical reactions between the repository constituents and the barrier materials. Because the corrosion and leaching processes are treated by empirical relationships, the chemistry is buried in the empirical rate factors. Hence, it is not clear what is taken into account.

*Page numbers in Sec. 3.27 are from ONWI-452.

Finally, it appears that the entire theory section needs careful technical editing. In Sec. 7, for example, the following errors were noted:

1. At the top of page 147, a constraint equation should appear but only an expression is given.
2. At the bottom of page 149, the term "mass accumulation," which implies an integration, is used whereas the word equation suggests only process rates.
3. In Eqs. 7.1-9, a sign separating two terms is missing.
4. In Eqs. 7.1-11 and 7.2-2, parentheses are missing.
5. In Eq. 7.2-4, parentheses are missing from two terms.
6. The terms "leach rate coefficient for diffusion" and "leach rate coefficient for dissolution" require explanation.

3.27.5 Code Design Review

ONWI-452 lists code inputs, outputs, and methods of solution for each of the process model codes. The input data consist of waste package design data, empirical data for various process rates, radio nuclide inventory and heat generation rate data, and boundary condition data for the waste-package/repository interface. The availability of the empirical rate data for the various corrosion processes seems uncertain, both because of the extent of the data required and because of the uncertainty of applicability of what are often short-term data to long-term processes. As noted in ONWI-452, short-term data may indicate that certain package materials are not subject to pitting or crevice corrosion. Yet, in the long term, such processes may arise and could lead to catastrophic failure of barriers. Radionuclide and heat input data are rather readily available from runs of ORIGEN2 or similar codes.

Specification of the time-dependent boundary conditions is probably the input requirement posing the greatest difficulty. This information will probably only be available through the operation of near-field repository heat transfer, fluid transport, and mechanical stress codes, whose input requirements will also be difficult to satisfy. How the boundary conditions at the interface will be handled will need clear definition in view of the intrinsically coupled nature of the waste-package/repository system.

3.27.6 Verification

Two types of verification were performed for each of the five process models of the WAPPA code. First, the results of hand calculations performed for simple problems were compared with the results of executing each of the process models and their submodels in a stand-alone fashion. All results agreed to within the accuracy of the hand

calculations. Second, using a complex 17-barrier waste package test problem, the entire integrated WAPPA code was executed and the results compared with the results obtained by manually feeding the input data obtained from the integrated WAPPA package code into the process models executed in the stand-alone mode. Comparisons again were very good, indicating that the integrated WAPPA code properly transmitted data to and from each process model during each time step. Three or four separate time steps tended to be used for this comparison.

For example, the radiation process model comprises four linked submodels -- source, attenuation, damage, and radiolysis. Computations performed by each of these submodels were checked with hand calculations, but only the results of the numerical integration performed by the attenuation submodel were reported in ONWI-452. These results compared very well with the results of the hand calculations. The integrated WAPPA code was then executed for the complex 17-barrier test problem mentioned above. The results were compared at three different time steps with the results of the radiation process model code operated in a stand-alone fashion by simulating input data from the integrated WAPPA code at the three time steps. The results verified that the radiation process model code was properly integrated into the entire WAPPA code.

The thermal process model contains temperature and heat flow algorithms, which were verified by comparing the results of hand calculations with those from code runs in the stand-alone mode. The 17-barrier test problem was used for this purpose. Predicted temperatures and heat flows from the stand-alone code and from the hand calculations were in good agreement for the one simulation time used ($t = 0$). Predicted temperatures and heat flows from the stand-alone code and from the integrated WAPPA code were in good agreement for the four simulation times used ($t = 0, 1, 100, \text{ and } 1000 \text{ years}$). Correct solutions for conductive and radiative heat transport across individual annuli over a range of material properties were verified. Logic options for various types of heat flow through the various barrier materials were also checked. Only temperature-independent properties for conductive and radiative heat transport were checked. Temperature-dependent convective heat transport was also checked.

The mechanical process model code was verified through a series of stand-alone and integrated system tests. Ten test cases compared hand calculations with stand-alone code runs. For example, waste-package-element stress fields were verified for radial and axial pressure loadings, thermal gradients, and residual stresses caused by initial displacement. The code correctly treats a fractured portion as an incompressible fluid. The system-integrated test demonstrated that (1) material properties are degraded as shown by radiation damage information from the radiation process model, (2) temperature gradients leading to thermal stresses are properly transferred from the thermal process model, and (3) the corrosion process model properly passes updated barrier thicknesses. Other details regarding integrated system performance were also verified.

The corrosion process model code contains many logic options and tracking/flagging variables. These options and variables, as well as the results of calculations using the simple algebraic expressions in the code, were verified by hand calculations. System integration testing indicated that the interfacing of data between this process code and the entire WAPPA code is correct.

The leach model tests used comparisons with hand calculations to verify the coding of the leaching, diffusion, and backfill equations and solution methods. Integrated system tests verified the interface between the WAPPA system and the leach process model code.

One point of uncertainty remains in the code verification procedure; namely, how do we know whether the integrated system code has been fully verified? That is, under the concerted action of all of the processes, are the various barriers breached when they are supposed to be, and is the effect of each breach properly handled in subsequent time steps by all of the process models? The answers to these questions are not easy to extract from the documented verification tests of each of the WAPPA process model codes. A clearer demonstration is needed that the integrated system has been verified.

3.27.7 Validation

No validation exercises have been documented.

3.27.8 Proposed ONWI Application

According to ONWI (1983), two applications of WAPPA are planned: (1) corrosion analyses of metallic barriers surrounding the waste form and (2) assessment of leach rates. WAPPA is designed specifically for these proposed applications. The corrosion process model embedded in WAPPA actually consists of several submodels of individual corrosion processes. WAPPA also contains a leach process model for estimating the flux of nuclides at the waste-package/repository interface. The effects of radiation and thermal output from the waste form on the corrosion and leaching processes are included in the WAPPA codes. However, certain processes that may be important are not considered (see Secs. 3.27.1 and 3.27.2).

3.27.9 Relationship of Model to Other Codes

Although WAPPA is a stand-alone code, it requires input data on nuclide inventories and heat generation rates for specific waste forms (and the irradiation histories of their constituents) from a source code like ORIGEN2. WAPPA contains a leach model that can provide leachate fluxes at the waste-package/repository interface, and these data can be used directly by geochemical and radionuclide transport codes like PHREEQE, EQ3/EQ6, and SWENT. SWENT, however, contains its own leachate model, which can be used in place of the WAPPA leachate model. WAPPA also provides information on heat flow through the waste package, which can be used to drive thermal/mechanical codes and fluid/energy transport codes. In considering relationships to other codes, it should be borne in mind that WAPPA assumes cylindrical symmetry of both input and output data, and uses a swept-away boundary condition at the waste-package/repository interface.

Both fluid and heat flux boundary conditions must be specified at the waste-package/repository interface, necessitating the iterative operation of WAPPA and

appropriate transport codes. Simple transport codes like STAFLO and DOT can be used for this purpose. Codes like STAFAN, CFEST, SWENT, TRIPM, and FTRANS may be required for more complex simulations involving coupled processes (e.g, flow in fractured or deformed porous media; coupled fluid, energy, and radionuclide transport; and solute transport and adsorption).

Finally, the corrosion processes that are assumed in WAPPA to operate from the outside of the waste package inward begin only after the surface of the outer barrier has been wetted. Hence, the user must predict the time at which such wetting occurs.

3.27.10 Application of Code to Other Problems

No applications of WAPPA to other problems have been documented.

3.27.11 Suitability of Model for Salt Repository Application

Most of the barrier destruction processes modeled in WAPPA are expressed in terms of empirical constants. Of special concern in a salt repository are the various corrosion rates and radionuclide leach rates that would govern the life of the waste package during an invasion of concentrated brine solutions at various temperatures. To the extent that such empirical data exist, WAPPA is applicable to salt repositories. The code documentation does not address the availability of specific salt repository data.

3.27.12 Peer Review

No peer review of WAPPA has been documented.

3.27.13 References for Section 3.27

INTERA Environmental Consultants, Inc., *WAPPA: A Waste Package Performance Assessment Code*, prepared for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio, ONWI-452 (April 1983).

Office of Nuclear Waste Isolation, *Preliminary Performance Assessment Plan for a Nuclear Waste Repository in Salt*, Battelle Memorial Institute, Columbus, Ohio, unpublished manuscript (March 1983).

Silling, S.A., *Final Technical Position on Documentation of Computer Codes for High-Level Waste Management*, U.S. Nuclear Regulatory Commission Report NUREG-0856 (June 1983).

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